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2 **Title:** MARMIT: a multilayer radiative transfer model of soil reflectance to estimate surface soil moisture
3 content in the solar domain (400–2500 nm)

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23 **Keywords:** Remote sensing, Soil moisture content, Reflectance spectroscopy, Radiative transfer model, Spectral signature

24
25 **Highlights:**

- 26
27
 - A multilayer radiative transfer model of soil reflectance as a function of surface water content is developed
 - A new method of SMC retrieval is developed
 - SMC retrieval combines good accuracy and efficiency after a soil classification
 - The new method is compared to other SMC retrieval methods

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33 **Journal:** *Remote Sensing of Environment*

34
35 **Abstract**

36 Surface soil moisture content (SMC) is known to impact soil reflectance at all wavelengths of the
37 solar spectrum. As a consequence, many semi-empirical methods aim at inferring SMC from soil
38 reflectance, but very few rely on physically-based models. This article presents a multilayer radiative
39 transfer model of soil reflectance called MARMIT (multilayer radiative transfer model of soil
40 reflectance) as a function of SMC given on a mass basis and a method called MARMITforSMC to
41 estimate it from soil reflectance spectra. This model depicts a wet soil as a dry soil covered with a thin
42 film of water. It is used to assess SMC over seven independent laboratory datasets gathered from the
43 literature. A learning phase is required to link the thickness of the water film with the SMC. For that
44 purpose, a sigmoid function, the parameters of which are related to soil physical and chemical
45 properties such as porosity, grain size and mineralogy composition, is fitted. SMC can be inferred
46 with good accuracy (RMSE \approx 3%) if the learning step is applied soil by soil. The link between SMC

47 and water thickness actually depends on soil texture and chemical composition. If the soils are divided
48 into classes and if the learning phase is applied to a class, the RMSE slightly increases up to 5%.
49 Finally, MARMITforSMC provides lower RMSE than any other existing semi-empirical or
50 physically-based method.

51

52 **1. Introduction**

53 Soil water content (or soil moisture content, SMC) assessment is critical in agriculture, hydrology,
54 micrometeorology, defense, civil engineering, and other environmental fields (e.g., [Gardner, 2000](#);
55 [Robinson et al., 2008](#); [Vereecken et al., 2008](#); [Wang and Qu, 2009](#); [Ochsner et al., 2013](#)). In
56 agriculture, SMC is an indicator of soil sensitivity to wind erosion; it also provides information about
57 water infiltration, runoff and storage that helps monitor soil-water-plant conditions and manage
58 irrigation ([Glenn et al., 2009](#); [Yang et al., 2012](#)). Therefore, it is highly correlated with crop yield
59 estimation. In hydrology and meteorology, SMC plays an important role in flood prevention
60 ([Haubrock et al., 2008](#)), incident radiation distribution and, indirectly, temperature and evaporation
61 ([Khanna et al., 2007](#); [Patel et al., 2009](#)); thus it contributes to mass conservation and energy balance
62 calculation. In defense or homeland security, trafficability depends on surface characteristics
63 including SMC and can be key in succeeding military or humanitarian operations. Vehicle traffic is
64 easier on dry clay paths and, conversely, on wet sand paths. SMC is also increasingly examined in
65 planetary sciences: for instance, the reflectance of some Martian surfaces in the near-infrared presents
66 strong absorption features attributed to the presence of water in the regolith or in the minerals that
67 compose it (e.g., [Milliken and Mustard, 2005, 2007a,b](#); [Pommerol et al., 2009, 2013](#)). Last but not
68 least, water alters the background reflectance of a bare soil and the apparent mineral absorption depths
69 in the spectrum, therefore it affects classification accuracy. Determining soil moisture content from
70 reflectance measurements may be useful to quantify other information of interest such as mineralogy,
71 salinity, texture, organic matter content or roughness (e.g., [Ben Dor et al., 2002](#); [Whiting, 2004](#);
72 [Bogrekci and Lee, 2006](#); [Minasny et al., 2011](#); [Rienzi et al., 2014](#); [Rodionov et al., 2014](#); [Zu et al.,](#)
73 [2016](#); [Marion and Carrère, 2018](#)).

74 There are three main types of soil water: (1) hydration (absorbed) water incorporated into the
75 lattice of minerals; (2) hygroscopic (adsorbed) water bound to soil particles, including soil organic
76 matter, due to the attraction between surface electrical charges and water molecules; (3) free water
77 covering the minerals, occupying the pores and moving through the soil by gravity and capillary
78 forces.

79 Soil water content generally refers to mass or volumetric water content, both expressed as a
80 fraction. As stated by [Stafford \(1988\)](#) or [Petropoulos et al. \(2013\)](#), there is no conventional method to
81 determine SMC. It is measured either in the laboratory with gravimetric and thermogravimetric
82 methods or in the field using, for example, portable neutron probes, time domain reflectometry (TDR)
83 or capacitance probes. Such measurements are reliable, but their footprint is limited to a few square
84 meters at most. Moreover, soil water content abruptly varies both in space and time due to the spatial
85 variability of soil physical properties and to the discontinuous nature of rainfall. All these methods
86 may be expensive and laborious to implement, especially at a fine spatial sampling interval, when a
87 large number of measurements are required.

88 Remote sensing can provide data at different spatial resolutions at reasonable costs. Moreover, it is
89 a non-destructive and non-invasive method. Most researches have focused on the measurement of the
90 backscattering coefficient and the brightness temperature in the microwave domain ([Njoku and
91 Entekhabi, 1996](#); [Das et al., 2008](#); [Mladenova et al., 2014](#)) that allow determining the volumetric
92 water content in the first centimeters, especially at lower frequencies ([Tabatabaenejad et al., 2015](#)).
93 But it often requires extra information about the soil dielectric constant or the surface roughness. In
94 the solar domain (400-2500 nm), light penetration in soil varies from a few micrometers to a few
95 millimeters depending on the wavelength and the soil type. Remote sensing offers the possibility to
96 determine moisture of the topmost layer of the soil with much higher spatial resolution ([Sadeghi et al.,
97 2017](#)) and may be an indicator of moisture below in some unique profiles.

98 Water spectroscopy is well known but still complex: the main absorption features of liquid water
99 occurring in the infrared result from vibrational transitions involving various overtones and
100 combinations of three fundamental vibrational transitions at 2870 nm (asymmetric O–H stretching),

101 3050 nm (symmetric O–H stretching), and 6080 nm (O–H bending). In the shortwave infrared, two
102 major water absorption peaks centered at 1470 nm and 1900 nm, and two minor absorption peaks
103 centered at 970 nm and 1200 nm, are observed. Smaller peaks and shoulders can be found in the
104 visible-near infrared at 514 nm, 606 nm, 660 nm, 739 nm, and 836 nm (Eisenberg and Kauzmann,
105 2005; Wozniak and Dera, 2007). The dominant effect of water on soil optical properties is an overall
106 decrease in spectral reflectance with increasing soil moisture. Idso et al. (1975) provided empirical
107 evidence that soil albedo decreased linearly with soil moisture, but subsequent studies have
108 challenged this view (Bowers and Hanks, 1965; Bedidi et al., 1992; Muller and Décamps, 2001).
109 Indeed, as is common in optics, nonlinear phenomena induce more pronounced absorption features in
110 the absorption bands of water than any others. For high SMC, soil reflectance may even increase with
111 moisture due to specular reflection (Neema et al., 1987; Liu et al., 2002). That critical point, which
112 seems to correspond to the field capacity, strongly depends on soil type (Liu et al., 2002). Soil
113 reflectance is controlled by many other factors such as texture, mineralogy, organic matter, and
114 surface roughness (e.g. Clark and Roush, 1984; Baumgardner et al., 1985; Okin and Painter, 2004;
115 Stenberg et al., 2010; Ben-Dor, 2011).

116 Numerous experiments have measured soil reflectance variation as a function of soil moisture in
117 the visible (VIS, 0.4-0.7 μm), in the near-infrared (NIR, 0.7-1.0 μm), in the shortwave-infrared
118 (SWIR, 1.0-3.0 μm) (e.g., Bowers and Hanks, 1965; Skidmore et al., 1968; Planet, 1970; Idso et al.,
119 1975; Twomey et al., 1986; Ishida et al., 1991; Liu et al., 2002; Haubrock et al., 2008), and more
120 recently, in the midwave-infrared (MWIR, 3.0-8.0 μm) and longwave-infrared (LWIR, 8.0-12.0 μm)
121 (e.g., Van Bavel et al., 1976; Narayanan et al., 1993; Bishop et al., 1994; Mira et al., 2007;
122 Lesaignoux et al., 2013). Many empirical methods link SMC and reflectance. They include spectral
123 indices (e.g., Levitt et al., 1990; Bryant et al., 2003; Khanna et al., 2007; Haubrock et al., 2008; Gao et
124 al., 2013), statistical relationships (e.g., Lesaignoux et al., 2013; Yin et al., 2013), multivariate
125 analysis (Mouazen et al., 2006), wavelet analysis (Peng et al., 2013) and exponential functions
126 (Muller and Décamps, 2001; Liu et al., 2002; Lobell and Asner, 2002; Whiting et al., 2004; Kaleita et
127 al., 2005; Sun et al., 2007; Somers et al., 2010; Verpoorter et al., 2014; Zhang et al., 2014). Such

128 methods have been applied to reflectance spectra and their successive derivatives, and to continuum-
129 removed spectra. However, most of them are not universal because they have been calibrated over a
130 limited range of soil types and knowledge of parameters such as soil density or porosity may be
131 required.

132 Very few methods relying on physically-based models have been developed. In the 1920s,
133 [Ångström \(1925\)](#) proposed a simple model where a wet soil is regarded as a dry soil covered with a
134 thin film of liquid water. This model derives the albedo of a wet soil by calculating the multiple
135 reflections between the two media based on Snell's law. [Lekner and Dorf \(1988\)](#) improved the
136 Ångström model by using the Fresnel coefficients instead of Snell's law. [Bach and Mauser \(1994\)](#)
137 introduced the Beer-Lambert-Bouguer law to account for light absorption in the water layer and
138 extended the model to the VIS-SWIR. More recently, [Kimmel and Baranoski \(2007\)](#) published a ray
139 tracing model called SPLITS (spectral light transport model for sand) and [Sadeghi et al \(2015\)](#)
140 proposed a model based on the Kubelka-Munk two-flux radiative transfer model. However, SPLITS
141 requires information on the soil that is somewhat difficult to access, high computing resources, and it
142 does not allow retrieving the SMC. As for the Sadeghi model, it only works at some wavelengths,
143 which reduces its field of application (see [Section 4.3](#)).

144 In this article, we improve the Bach model ([Bach and Mauser, 1994](#)) which appears to efficiently
145 estimate the surface SMC ($r^2 = 0.88$) but which has not been validated or improved in the literature
146 for the past twenty years. The equations underlying the multilayer radiative transfer model of soil
147 reflectance (MARMIT) are detailed, and the validation datasets are presented. Then, a method to
148 retrieve SMC called MARMITforSMC and based on a logistic function is introduced and compared to
149 other statistical or semi-empirical methods.

150

151 **2. Model and datasets**

152

153 **2.1 Description of MARMIT**

154 MARMIT mimics a wet soil as a dry soil covered with a thin film of water (Fig. 1). Such an
 155 approach is naturally a simplified version of reality, as the geometry of water films within soils is
 156 much more complex (Tuller et al., 1999). A fraction of light is transmitted from the air (medium 1) to
 157 the water layer (medium 2) with a transmissivity t_{12} . Another fraction is reflected to the air. The
 158 reflectivity at the interface is $r_{12} = 1 - t_{12}$. Then light is diffusely scattered through internal multiple
 159 reflections between the liquid-soil interface (R_d) and the liquid-air interface (r_{21}). These multiple
 160 reflections increase the probability of light absorption by soil particles and explain why a wet soil
 161 appears darker than a dry soil. The fraction of light that is not reflected back to the soil is transmitted
 162 from the water to the air (t_{12}).

163

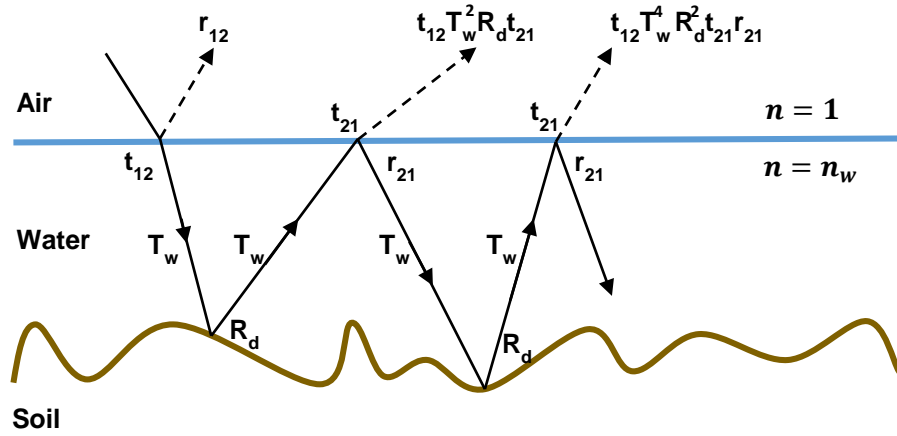


Fig. 1. Thin liquid water layer over a rough surface. Medium 1 is air and medium 2 is water. r_{ij} and t_{ij} are the reflectivity and transmissivity at the interface between the media i and j , T_w is the transmittance of the water layer, R_d the reflectance of the dry soil. n_w is the refractive index of water, that of air being assumed to be 1. All these physical quantities are wavelength dependent.

164

165 MARMIT results from a series of improvements of an approach initiated by Ångström (1925),
 166 continued by Lekner and Dorf (1988) half a century later, and by Bach and Mauser (1994) a few years
 167 later. In the first two papers, water absorption is assumed to be negligible in the VIS-NIR and the total
 168 absorptance of a wet soil is calculated as

169

$$A_{wSL} = \frac{t_{12}A_d}{1 - r_{21}R_d} \quad (1)$$

170

171 where $A_d = 1 - R_d$ is the absorptance of the dry soil, t_{12} the transmissivity at the air-water interface
 172 and r_{21} the reflection coefficient at the water-air interface. Both are calculated by the Fresnel
 173 equations for unpolarized light. t_{12} depends on the incidence angle θ_i formed between the normal and
 174 the incident ray and on the relative refractive index n defined as the ratio of the refractive index of
 175 pure liquid water (n_w) to the refractive index of the air ($n_a = 1$): $n = n_w/n_a = n_w$. Ångström
 176 (1925) assumes that light exiting the water layer lies within a cone of a given angle while Lekner and
 177 Dorf (1988) consider a diffuse light. The latter consequently calculate r_{21} by integrating the
 178 reflectivity over the entire hemisphere (Stern, 1964):

$$r_{21} = 1 - \frac{1}{n^2}(1 - r'_{12}) \quad (2)$$

181 with

$$r'_{12} = \frac{3n^2 + 2n + 1}{3(n + 1)^2} - \frac{2n^3(n^2 + 2n - 1)}{(n^2 + 1)^2(n^2 - 1)} + \frac{n^2(n^2 + 1)}{(n^2 - 1)^2} \log n - \frac{n^2(n^2 - 1)^2}{(n^2 + 1)^2} \log \frac{n(n + 1)}{n - 1} \quad (3)$$

184 The hypothesis of a nonabsorbing water layer is invalid in the SWIR. Bach and Mauser (1994)
 185 calculate its transmittance T_w with the Beer-Lambert law: $T_w = \exp(-\alpha_B L)$ with α_B the specific
 186 absorption coefficient of *in situ* water determined empirically [m^{-1}] and L the thickness of the water
 187 layer [m]. Therefore, the reflectance of a wet soil is written in the form

$$R_{wsB} = (1 - A_{wsL}) \exp(-2\alpha_B L) \quad (4)$$

190 with A_{wsL} the total absorptance of a wet soil defined in Eq. (1). The factor 2 is because the light ray
 191 crosses twice the water layer. Considering that the soil surface may be a patchwork of wet and dry
 192 areas, Bach (1995) introduced an efficiency term ε that accounts for the fraction of wet soil:

$$R_{modB} = \varepsilon \times R_{wsB} + (1 - \varepsilon) \times R_d \quad (5)$$

195 $\varepsilon = 0$ means that the soil is dry and $\varepsilon = 1$ that it is covered with a film of water over its whole
 196 surface.

197 In MARMIT the transmittance of light through the water layer is taking into account along the path
 198 of the ray (Fig. 1). The expression for the total reflectance of the water/soil system can be derived by
 199 summing the amplitudes of successive reflections and refractions at the top of the water layer:

$$200 \quad R_{ws} = r_{12} + t_{12}T_w^2R_d t_{21} + t_{12}T_w^4R_d^2 t_{21}r_{21} + \dots \quad (6)$$

202 Eq. (6) can be easily factorized in

$$203 \quad R_{ws} = r_{12} + t_{12}t_{21}R_d T_w^2(1 + r_{21}R_d T_w^2 + r_{21}^2R_d^2 T_w^4 + \dots) \quad (7)$$

205 The expression in brackets is a geometric series of general term $x = r_{21}R_d T_w^2$ that converges to $\frac{1}{1-x}$
 206 if $|x| < 1$. So we obtain

$$207 \quad R_{ws} = r_{12} + \frac{t_{12}t_{21}R_d T_w^2}{1 - r_{21}R_d T_w^2} \quad (8)$$

209 with $T_w = \exp(-\alpha L)$, α the absorption coefficient of pure liquid water provided by Palmer and
 210 Williams (1974). If the soil is dry, the transmission-related parameters t_{12} , t_{21} and T_w are 1 and the
 211 reflections r_{12} and r_{21} are 0, then $R_{ws} = R_d$. MARMIT also introduces an efficiency term ε like in
 212 Eq. (5),

$$213 \quad R_{mod} = \varepsilon \times R_{ws} + (1 - \varepsilon) \times R_d \quad (9)$$

215 In the following, the term r_{12} is ignored because the diffuse radiation is negligible for our
 216 laboratory measurements and none of the measurements described hereafter have been acquired in the
 217 specular direction while the water layer is assumed to be flat. In conclusion, MARMIT is physically
 218 more consistent than the previous models because the coupling between the multiple reflections and
 219 the absorption of light in the water layer is more realistic. The differences between the models
 220 presented above are summarized in Table 1.

Author	Lekner and Dorf (1988)	Bach (1995)	MARMIT
Physical variable	absorptance	reflectance	reflectance
Expression	A_{wSL}	R_{wsB}	R_{ws}

Equation	$\frac{t_{12}A_d}{1 - r_{21}R_d}$	$(1 - A_{wSL})\exp(-2\alpha_B L)$	$\frac{t_{12}t_{21}R_dT_w^2}{1 - r_{21}R_dT_w^2}$
Remark	Summation of the absorptances above the water layer; no light absorption in the water layer	Transmittance of light in the water layer accounted for and multiplied by $1 - A_{wLD}$; empirical absorption coefficient of water	Transmittance of light in the water layer directly added in the path of the ray; absorption coefficient of pure liquid water

Table 1. Summary of every model described in this section.

222

223 2.2 Datasets

224 MARMIT was tested on a database gathering six datasets published in the literature, plus a new
225 one generated in the frame of this study (Table 2). They are, in order of publication year, Liu02 (Liu
226 et al., 2002, 2003), Lob02 (Lobell and Asner, 2002), Whit04 (Whiting, 2004; Whiting et al., 2004),
227 Les08 (Lesaignoux, 2010; Lesaignoux et al., 2013; Fabre et al., 2015), Mar12 (Marcq, 2012), Phil14
228 (Tian and Philpot, 2015a,b), and Bab16 (this article). They represent a total of 217 soil samples.
229 Ideally the number of SMC levels would cover the full range of soil moisture variation and textural
230 information about the soil samples would be available. The incompleteness of the datasets does not
231 allow completely validating MARMIT, analyzing its performance, and explaining the results. For
232 instance, Whit04, Lob02 and Mar12 have many SMC levels but little textural information about the
233 soil samples. The latter is available in Liu02 but there are only four SMC levels. The new Bab16
234 dataset includes enough SMC levels with relevant information on soils.

235

Dataset	N	SMC		Drying protocol	Sieving	θ_i	Bulk density
		Number of levels	range				
Liu02	92	4	0-83 %	Oven-dried	2 mm	15°	0.98-1.88
Lob02	4	9 to 15	0-118 %	Oven-dried	2 mm	15°	0.64-1.54
Whit04	60	10 to 12	0-45 %	Air-dried	2 mm		0.88-1.36
Les08	32	6	0-87 %	Oven-dried	no	15°	
Mar12	9	25 to 30	0-50 %	Humidification	no	25°	
Phil14	3	97 to 205	0-45 %	Air-dried	2 mm	30°	0.95-1.53
Bab16	17	6 to 8	0-40 %	Oven-dried	2 mm	15°	

Table 2. Summary of the main information on the datasets. N is the number of soil samples, SMC is the soil moisture content, θ_i is the angle of the incident light.

236

237 The soil samples in Whit04 originate from two locations: fifteen come from Tomelloso (Castilla-
238 La Mancha, Spain) and as many from Lemoore (California, USA). Whiting et al. (2004) made two
239 replicates of each soil so that the dataset gathers sixty samples. The soils sampled in Lemoore belong

240 to three textural soil classes: clay loam, sandy clay loam, and silty clay loam; those sampled in
 241 Tomelloso also include three soil classes: loam, sandy loam, and silt loam. Organic matter content is
 242 low in both regions (< 2%). Soil mineralogy (CaCO_3 and SiO_2 contents) is provided for four soils
 243 from Tomelloso and five soils from Lemoore. Whiting et al. (2004) removed the reflectance between
 244 760 nm and 950 nm because of detector artifacts in that region. The textural information is available
 245 for the 92 soils of Liu02, the 32 soils of Les08, and 10 out of 17 soils of Bab16 (Fig. 2). Lob02
 246 includes four soils displaying various mineralogical compositions, amounts of organic matter, and
 247 porosities. Mar12 includes six different soils collected in the region of Reims (France). Three of them
 248 (soils 1, 2 and 4) have one replicate.

249

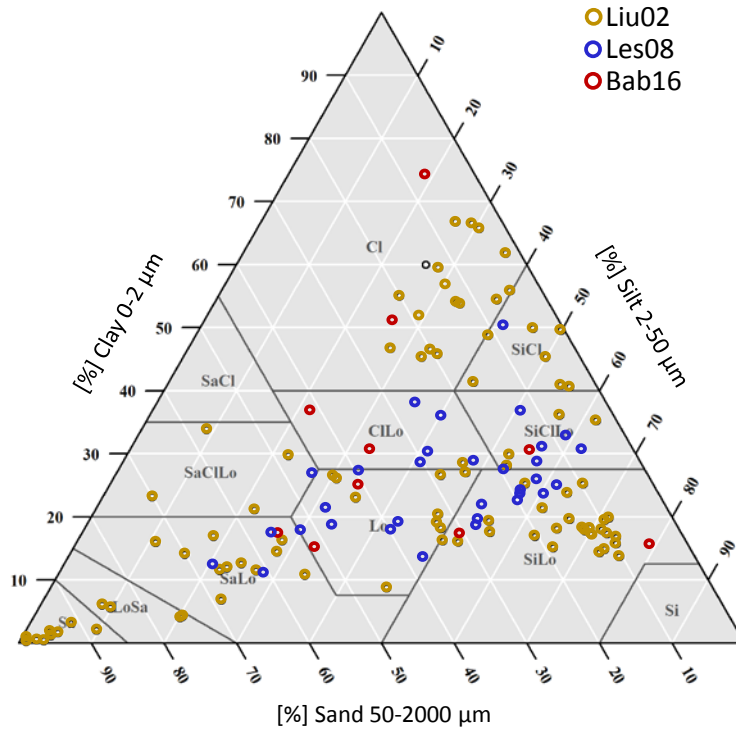


Fig. 2. Soil texture triangle showing the 12 major textural classes and particle size scales as defined by the USDA, for 134 soils of three datasets (Liu02, Les08, and Bab16).

250

251 Soil moisture content was most of the time expressed as a weight percent (SMC_g):

252

$$\text{SMC}_g = \frac{M_{ws} - M_{ds}}{M_{ds}} = \frac{M_{H_2O}}{M_{ds}} \quad (10)$$

253

254 with M_{ws} [g] the mass of wet sample, M_{ds} [g] the mass of dry sample, and M_{H_2O} [g] the mass of
 255 water. Sometimes it was expressed as a volumetric percent (SMC_v):

256

$$SMC_v = \frac{V_{ws} - V_{ds}}{V_{ds}} = \frac{V_{H_2O}}{V_{ds}} \quad (11)$$

257

258 with V_{ws} [cm^3] the volume of wet sample (dry soil and water-filled pores), V_{ds} [cm^3] the volume of
 259 dry sample, and V_{H_2O} [cm^3] the volume of water. SMC_g and SMC_v are related by the dry bulk density
 260 of the sample (Lobell and Asner, 2002):

261

$$SMC_v = \frac{V_{H_2O}}{V_{ds}} = \frac{M_{H_2O} \times d_{ds}}{M_{ds} \times d_{H_2O}} = SMC_g \times \frac{d_{ds}}{d_{H_2O}} \quad (12)$$

262

263 with d_{H_2O} [g.cm^{-3}] the density of water (~ 1) and d_{ds} [g.cm^{-3}] the dry bulk density of the sample.
 264 Because densities of the soils were not available for every dataset, SMC_g has been used in this study
 265 instead of SMC_v . In the following, if nothing is specified, the SMC will refer to the definition of SMC_g .

266

The experiments vary somewhat so we refer the reader to the original articles for spectrometer
 267 setup and moisture measurement protocol. Most of the data were acquired with an ASD FieldSpec
 268 spectroradiometer (Analytical Spectral Devices, Inc.) except for Whit04 where a Cary 5E
 269 spectrophotometer (SpectraLab Scientific, Inc.) was used. All the datasets but Mar12 were acquired
 270 according to the same protocol: the soil sample is sieved, put into a Petri dish with a radius of about 5
 271 cm, moistened up to saturation (except for Liu02 where the saturation stage is exceeded) and then
 272 dried. At regular intervals during drying, the soil samples are weighed in order to assess SMC and
 273 their reflectance spectrum is recorded. Mar12 was obtained in a somewhat different way since the soil
 274 samples were not sieved and moistened after drying. Moreover, they were put into pie plates with a
 275 radius around 25 cm.

276

All the datasets associate a reflectance spectrum with a water content value measured
 277 concomitantly. Since reflectance varies with the angle of the incident light θ_i , precautions will be
 278 taken when comparing Mar12 and Phil 14 to the other datasets. Fig. 3 shows the evolution, as a
 279 function of water content, of the reflectance of a clay soil, a loamy soil, and a sandy soil picked at the
 280 vertices of the texture triangle.

281

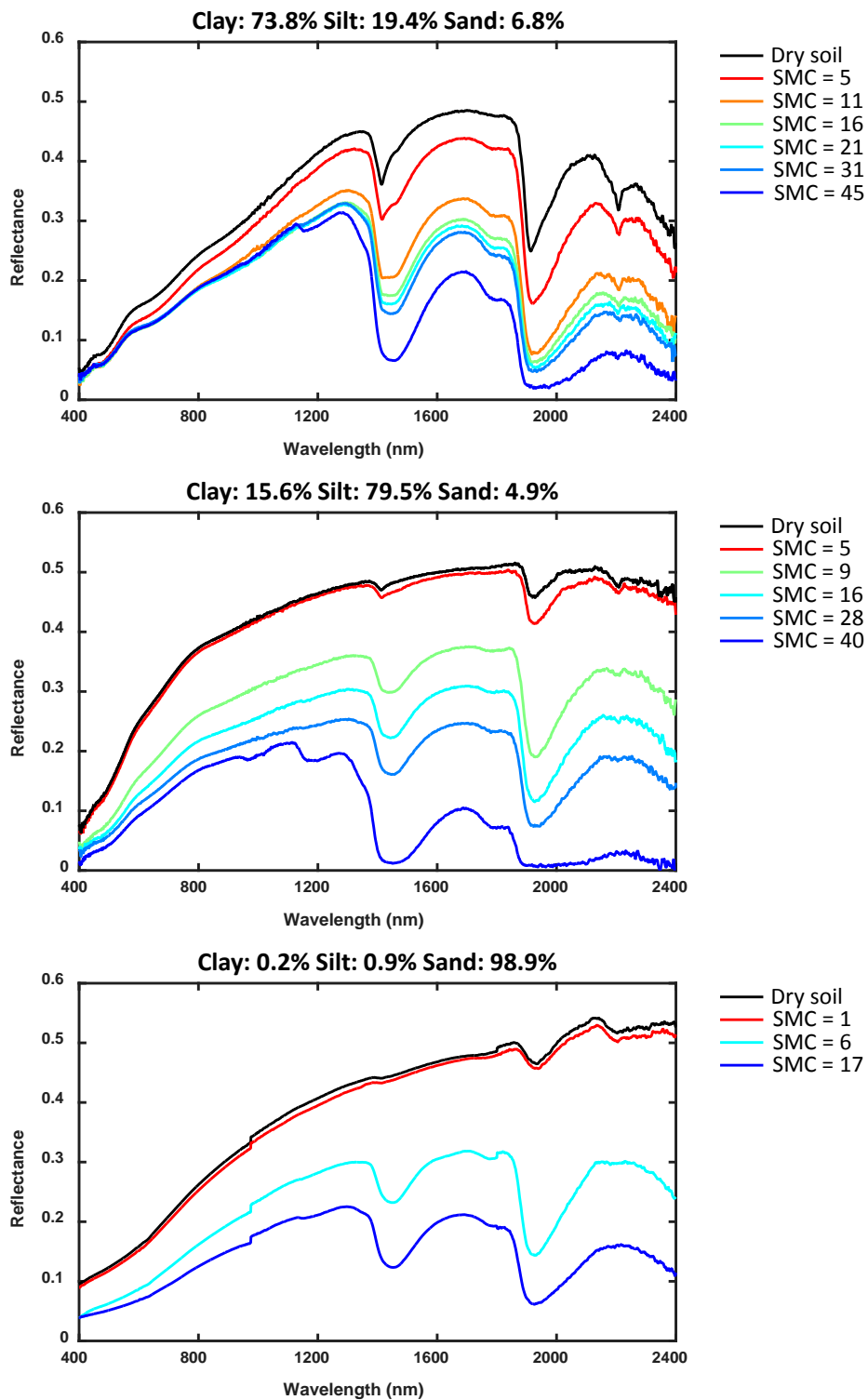


Fig. 3. Reflectance spectra and their associated SMC_g (g/g). (top) Clay soil 724 *Lebna57* in Bab16, (middle) loamy soil *Luvisol 208Te* in Bab16 and (bottom) sandy soil 76 in Liu02.

282

283 The clay soil made of very fine particles holds greater amounts of water and has greater porosity
 284 than coarser soils, so the SMC at saturation is higher (Fig. 3, top). Conversely, the sandy soil made of
 285 large particles has a lower porosity; it rapidly reaches saturation (Fig. 3, bottom). Finally, the SMC of
 286 the loamy soil at saturation is in-between (Fig. 3, middle).

287

288 2.3 The MARMITforSMC approach

289 The method for retrieving soil moisture content with MARMIT called MARMITforSMC involves
290 three steps (Fig. 4):

291 (1) Inversion step: the water thickness L and the efficiency ε are estimated by model inversion
292 (Eq. (14)). One can note that the reflectance of the dry soil is needed to infer the reflectance of
293 a wet soil.

294 (2) Calibration step: a statistical relationship is established between the mean water thickness
295 (mean light path) defined as $\varphi = L \times \varepsilon$ and the measured SMC. Here we use φ instead of L
296 because, for very small SMC, ε changes slowly in comparison to L which can vary very
297 quickly.

298 (3) Assessment step: SMC is retrieved by applying the relation found in the calibration step and
299 compared with the measured values.

300

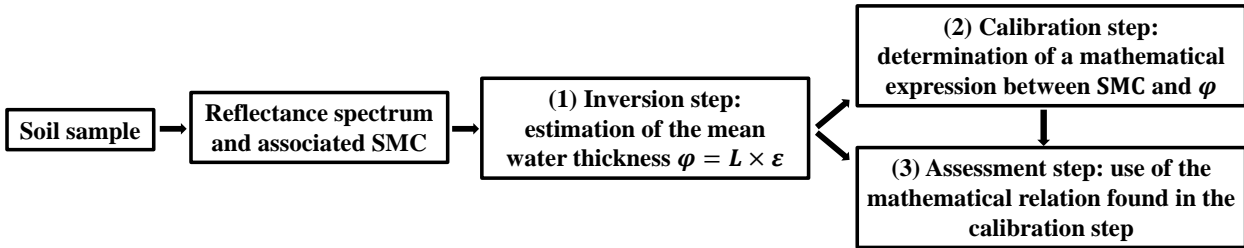


Fig. 4. Flowchart representing the overall MARMITforSMC method used in this study.

301

302 3. Results

303 The root-mean-square error (RMSE) that measures the difference between the measured and
304 estimated values of SMC was chosen to compare the efficiency of the various regressions and models:

305

$$306 \quad RMSE = \sqrt{\frac{\sum_{i=1}^N (SMC_i^{meas} - SMC_i^{est})^2}{N}} \quad (13)$$

307

308 where SMC_i^{est} is the estimated SMC for the soil sample i , SMC_i^{meas} is the measured SMC, and N is
the number of SMC.

309

310 3.1 Inversion step

311 The inversion step is applied to all the samples. Model fitting is achieved by searching the best
 312 values of L and ε that minimize the merit function χ^2 thanks to the bounded simplex search algorithm,
 313 implemented in MATLAB (Nelder and Mead, 1965):

314

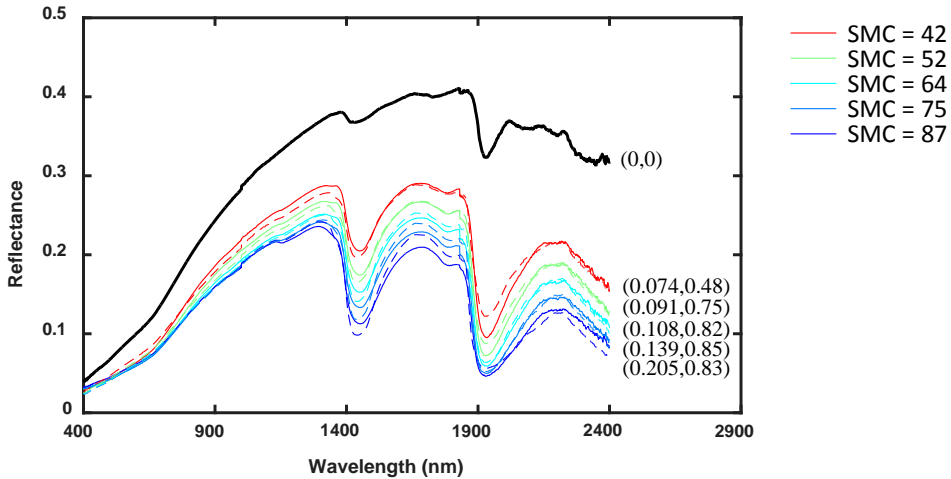
$$\chi^2(L, \varepsilon) = \sqrt{\frac{\sum_{\lambda_1}^{\lambda_2} (R_{meas}(\lambda) - R_{mod}(\lambda, L, \varepsilon))^2}{n_\lambda}} \quad (14)$$

315

316 with R_{meas} the measured reflectance at wavelength λ , R_{mod} the modeled reflectance described in Eq.
 317 (9) at wavelength λ , and n_λ the number of wavelengths. In our case, $\lambda_1 = 400$ nm and $\lambda_2 = 2400$ nm.

318 The fit is good for most of the soils ($r^2 > 0.95$, Fig. 5, top) but, when SMC is higher than 20%, the
 319 reflectance of some soils is overestimated by the model outside the water absorption bands and
 320 underestimated within these bands ($r^2 < 0.90$, Fig. 5, bottom). This misfit decreases if ε is
 321 unconstrained but we bounded it between 0 and 1 to keep a physical meaning.

322



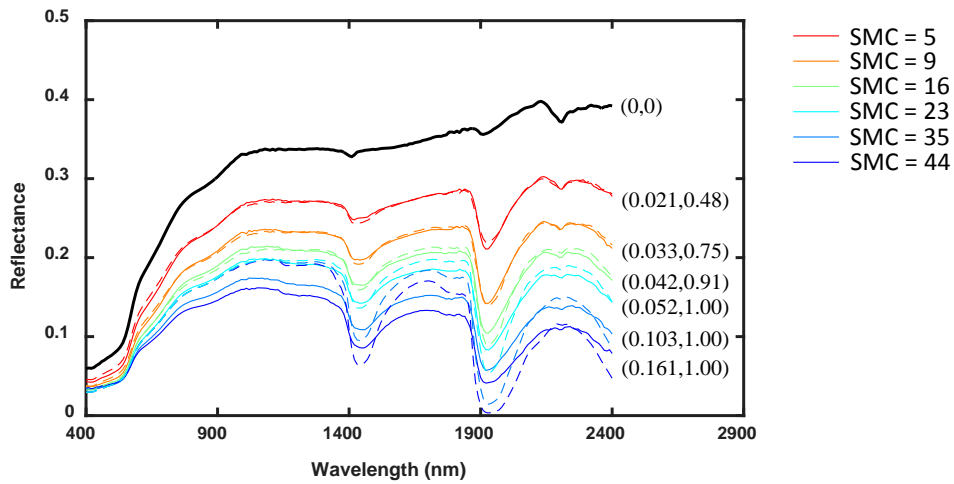


Fig. 5. Measured (solid line) and modeled (dashed line) reflectance spectra of two soils at various levels of soil water content: (top) *30PrairieB* in Les08 with SMC in weight percent ($\text{g.g}^{-1} \times 100$) and (bottom) *Entisol* in Lob02 with SMC in volumetric percent ($\text{cm}^3.\text{cm}^{-3} \times 100$). The retrieved parameters of the model are provided to the right of the curves (L, ϵ). L is in mm.

323

324 The RMSE between the measured and the modeled reflectance spectra of all soils of all dataset is
 325 generally lower than 2% except at 1900 nm, a major water absorption band (Fig. 6). Philpot (2010)
 326 suspects that part of this discrepancy is due to a change in the optical properties of the liquid phase of
 327 soil when water, that already contains dissolved organic matter and ions, is mixed with suspended
 328 mineral particles. Bach (1995), who empirically derived a specific absorption coefficient of water
 329 bound with soil, obtained a better fit with her model in the water absorption band at 1900 nm but
 330 applying this coefficient to every kind of soil is difficult to justify so we decided to use the specific
 331 absorption coefficient of pure liquid water (Fig. 6).

332

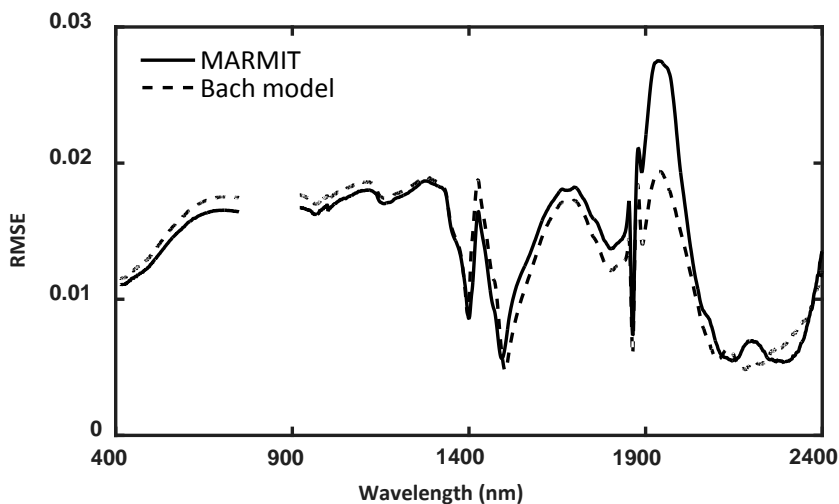


Fig. 6. Root-mean-square error (RMSE) between the soil spectra and two soil reflectance models, calculated for all the datasets.

333

334 3.2 Calibration and prediction steps

335 The calibration step consists in finding a mathematical expression relating the mean water
336 thickness (φ) to the soil moisture content (SMC). It is not possible to determine a unique relationship
337 valid for all soils of all datasets because the points are widely scattered (Fig. 7). The relationship
338 seems to depend on soil characteristics and measurement protocols: as an example the two white
339 quartz sands in Phil14 and Bab16, which are very bright, are distinct from the other soils. One also
340 notes that the soil samples of Mar12, which were wetted instead of being dried, display a relationship
341 shifted by about 0.1 mm on the right compared to the other soils. Tian et al. (2015b) mention that
342 water tends to stagnate on the surface of the soil during humidification so that a small amount of water
343 induces a significant change in reflectance. Conversely during drying, water and air are distributed
344 throughout the sample for most of the drying period, so that soil reflectance does not change much
345 when the sample is almost dry.

346

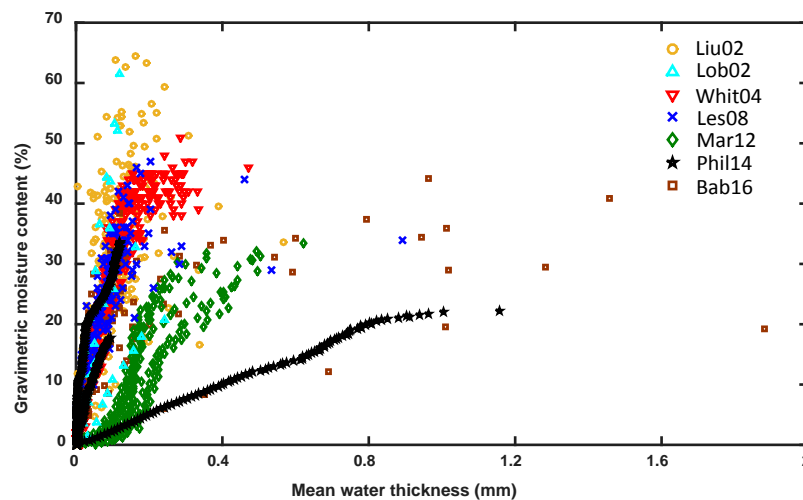


Fig. 7. Relationship between SMC_g and φ for all soils of all datasets.

347

348 Because no general relationship could be found, the soils were first studied separately and then
349 gathered into classes based on textural, mineralogical, and spectral properties.

350

351 3.2.1 Soil-by-soil calibration and prediction steps

352 Several models such as polynomials of degree one (Bach and Mauser, 1994; Bach, 1995), two or

353 three, as well as power functions have been tested to adjust the points relating SMC to φ . The S-shape
 354 curvatures observed for almost every soil suggest using a logistic function:

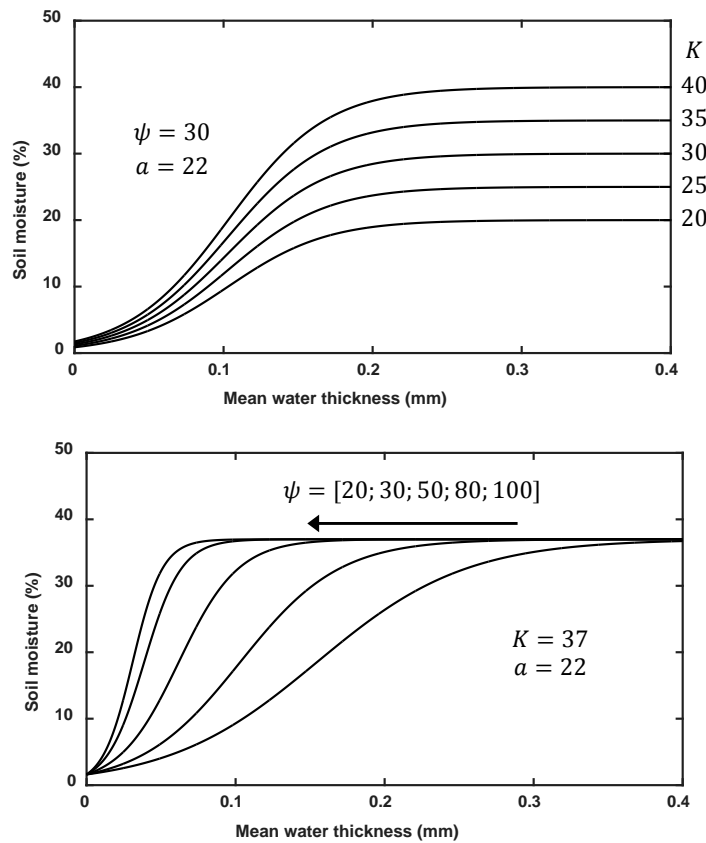
355

$$SMC = \frac{K}{1 + ae^{-\psi\varphi}} \quad (15)$$

356

357 with K the maximum value of the curve, ψ the steepness of the curve, and a a translation factor that
 358 moves the whole curve along the x-axis. A simple one-factor-at-a-time sensitivity analysis of the
 359 logistic function illustrates the effect of each parameter on the curve shape (Fig. 8). An increase in K
 360 induces an increase in the asymptote of the curve; an increase in a shifts the whole curve to the right;
 361 an increase in ψ increases the slope of the curve and shifts the inflexion point towards the smallest
 362 values of φ .

363



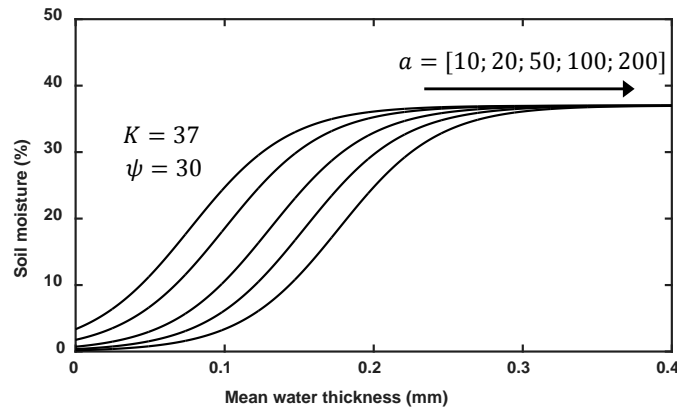
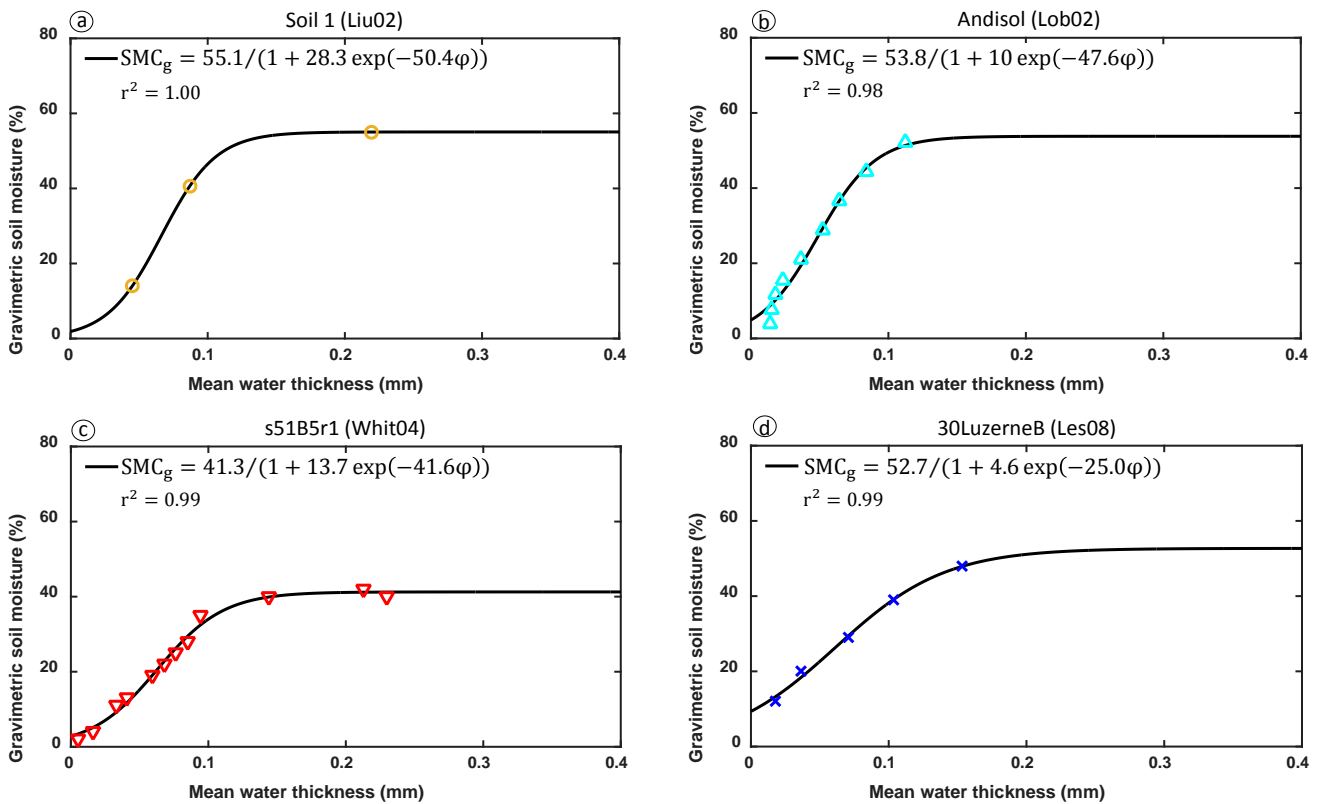


Fig. 8. Schematic trends of a logistic function. (top) K is variable, ψ and a are constant; (middle) ψ is variable, K and a are constant; and (bottom) a is variable, K and ψ are constant.

364

365 Fig. 9 shows that the logistic function explains very well the evolution of the SMC with φ for
 366 every soil. The relationship is not constrained: $\varphi = 0$ does not mean that the soil sample is dry but
 367 that there is no detectable water on the soil surface. Moreover a logistic function is strictly positive
 368 when the parameters K , ψ and a are positives. The function is then called a sigmoid function.

369



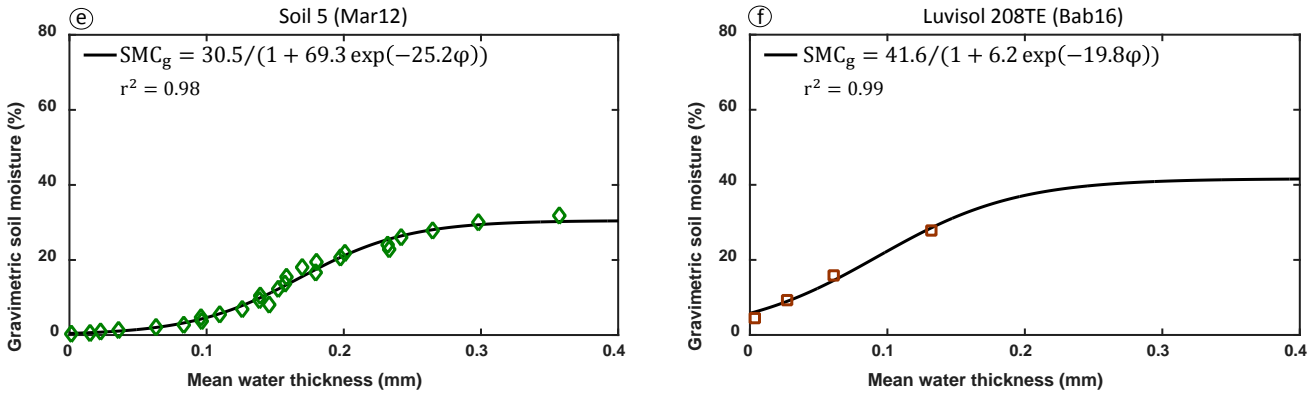


Fig. 9. Calibration step for six soils of six different datasets. Name of the soil in title and dataset in bracket.

370

371 Note that when K is at the maximum value of SMC, i.e., saturation, the soil pores are filled with
 372 water and the volumetric water content is nearly equal to the porosity. Since the volumetric and the
 373 gravimetric water contents can be calculated by Eq. (12), K may be related to the porosity of the soil.
 374 To validate this assumption, we plotted the maximum soil water content, i.e., the water content at
 375 saturation (SMCs), as a function of K (Fig. 10). In most cases, there is a correspondence between the
 376 two but K sometimes diverges from the bisector because of the limited range of soil moistures
 377 available in some datasets. If now we remove the soil samples containing less than six data points
 378 (twice the number of parameters in the sigmoid function), these two parameters are almost equivalent.

379

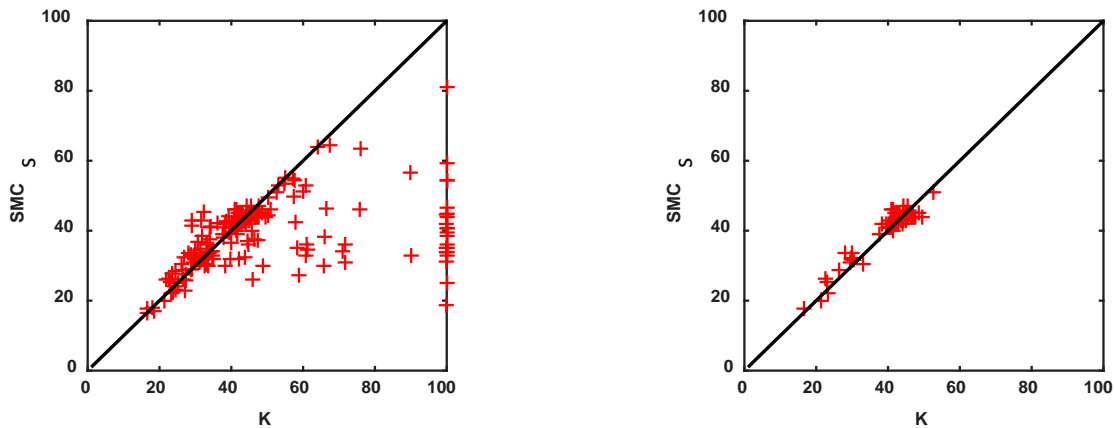


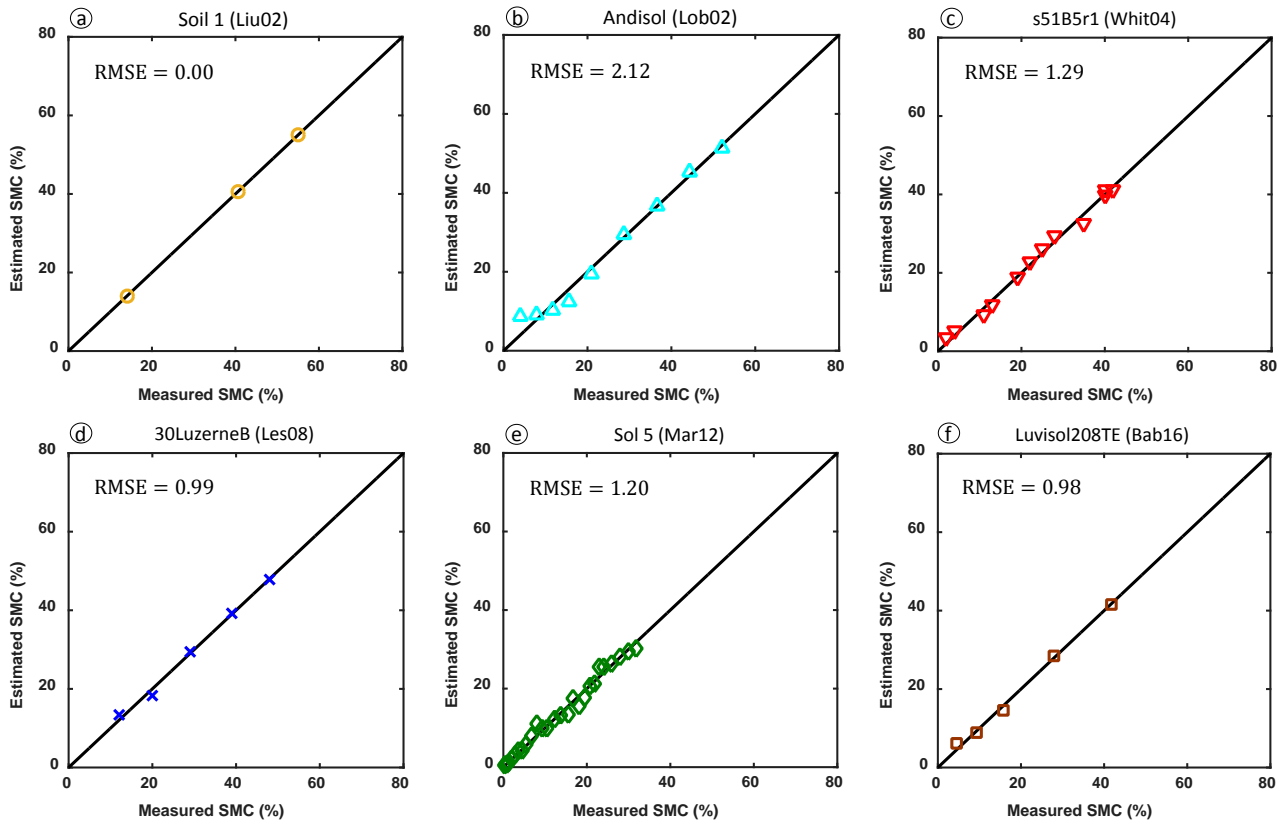
Fig. 10. Link between K and SMCs (left) for every soil of every dataset and (right) for the soils with more than six moisture content measurements.

380

381 If the values of φ determined during the inversion step are reinjected into the relationship found
 382 between SMC and φ , and if the measured and estimated soil moisture contents are compared, then
 383 excellent results are obtained ($RMSE < 3\%$). It proves that the soil-by-soil calibration is very

384 efficient (Fig. 11).

385



386 **Fig. 11.** Estimated vs measured SMC for the six soil samples used in the calibration step in the Fig. 9.

387

388 We used the replicates of the Whit04 dataset to test the soil-by-soil calibration and to validate the
389 method. A relationship has been adjusted between φ and SMC for thirty soil samples, leading to as
390 many calibration equations that have been applied to the replicates. The estimation error is generally
391 less than 5% and the RMSE 2.8% (Fig. 12). In comparison, the errors associated with field TDR
392 measurements are approximately 2.5% in volume percent of water (Walker et al., 2004).

392

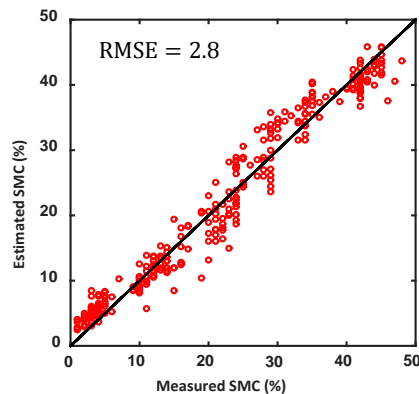


Fig. 12. Estimated vs measured SMC for the soils of the Whith04 dataset.

393

394 One of the advantages of remote sensing is a large spatial coverage, but detailed knowledge of the
395 nature of the investigated soils is barely available because they may change quickly in terms of texture
396 and structure from one spot to another. Therefore, an approach requiring a calibration relation
397 between SMC and φ for each soil hardly applies since there is no unique relation as shown in Fig. 7.
398 In order to fulfill operational requirements, we attempted classifying soils into groups. Several
399 techniques were used, based on soil physical, chemical and spectral characteristics.

400

401 **3.2.2 Class-by-class calibration and assessment steps: physical and chemical properties**

402 First, the effects of mineralogy and texture in the estimation of the relationship between SMC and
403 φ were investigated. To this end, we took advantage of the mineralogical information of the Whit04
404 dataset. The amount of calcium carbonate (CaCO_3) and silicon dioxide (SiO_2) in the Tomelloso soils is
405 quite variable, while there is no CaCO_3 and a constant amount of SiO_2 (~29%) in the Lemoore soils.
406 The relationship between SMC and φ is consequently more scattered for the first ($r^2 = 0.93$) (Fig.
407 13a) than for the second ($r^2 = 0.97$) (Fig. 13b). While the modification of the spectral properties of a
408 soil when moistened depends upon its mineralogical composition (Bedidi et al., 1992), it may
409 influence the parameters ψ and a of the sigmoid function. The soils of Les08 and Bab16 that contain
410 textural information were also investigated. We divided them into two groups: sandy soils for which
411 50% of the grain size is sand (larger than 0.05 mm and less than 2 mm) and clay soils for which 50%
412 of the grain size is clay (less than 2 μm). The relationship between SMC and φ is well fitted by the
413 sigmoid function in both cases, with high coefficients of determination (Figs. 13c and 13d).
414 Furthermore, the parameter K is lower for the sandy soils (46.2%) than for the clay and silt soils
415 (59.1%) in accordance with the fact that the porosity of the former is lower than that of the latter. This
416 is consistent with the hypothesis that the parameter K is related to this soil property. These results
417 show that our method can be generalized by making a preliminary soil texture and mineralogical
418 composition classification. Unfortunately, such information is seldom available.

419

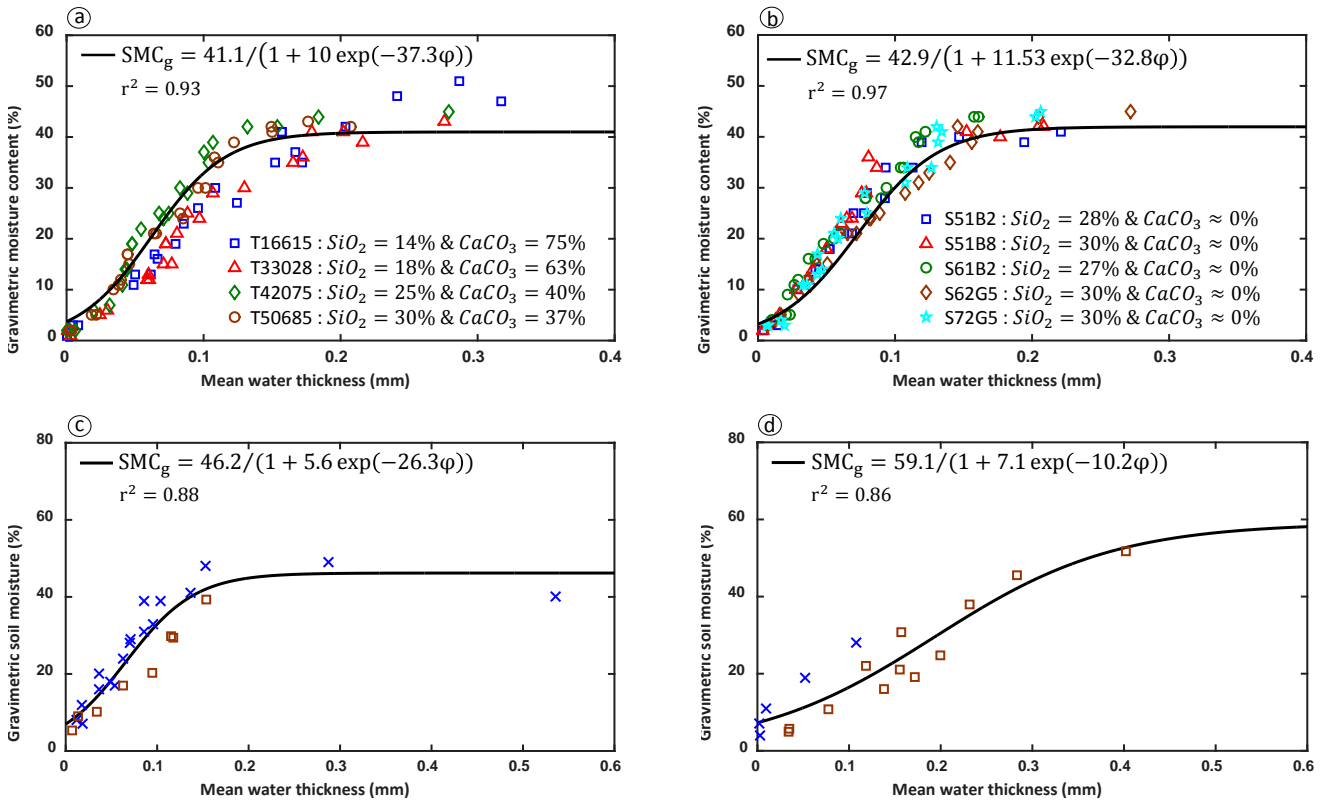


Fig. 13. Calibration phase for (a) four soils from Tomelloso and (b) five soils from Lemoore (Whit04 dataset). Calibration phase for (c) six sandy soils and (d) nine non-sandy soils of the Les08 (blue crosses) and Bab16 (brown squares) datasets.

420

421 3.2.3 Class-by-class calibration and prediction: spectral signatures

422 We investigated the classification method proposed by Lesaignoux et al. (2013) where the soils are
 423 grouped together on the basis of the shape of the dry soil reflectance spectrum in four wavelength
 424 ranges (VIS, NIR-SWIR, MWIR, and LWIR). The 32 soils were initially divided into nine groups but,
 425 in this study, groups 1 and 2 and groups 4 and 5 were merged together because the shape of their dry
 426 soil is identical in the VIS and NIR-SWIR and because our study is restricted to these domains.
 427 Moreover groups 3, 7, 8 and 9 which contain less than two soils were discarded. Finally we
 428 maintained three classes: class I (groups 1 and 2), class II (groups 4 and 5), and class III (group 6).
 429 Figs. 14a-d compare the sigmoid functions obtained on these three classes and on the whole dataset.
 430 Note that because some soils of Les08 are excluded from the three classes, some points of Fig. 14a do
 431 not appear in Figs. 14b-d. The r^2 values of 0.71, 0.84 and 0.98 for class I, II and III, respectively, are
 432 globally better than that of the whole dataset ($r^2 = 0.75$). The calibration equation of class III
 433 displays a very high coefficient of determination probably because all the samples have been collected
 434 in the same area (Camargue, France). The soils of class II that contain a maximum number of samples

435 have been divided into two sub-classes: one for the calibration and one for the validation (Figs. 14e-f).
 436 Soil moisture content is very well inferred thanks to that classification (RMSE = 5.1%) although the
 437 accuracy is worse compared to the soil-by-soil calibration, as expected. Nevertheless, the
 438 classification was based upon a visual method: it may introduce some mistakes and it is not suited for
 439 large datasets, so it cannot be applied to the whole database.

440

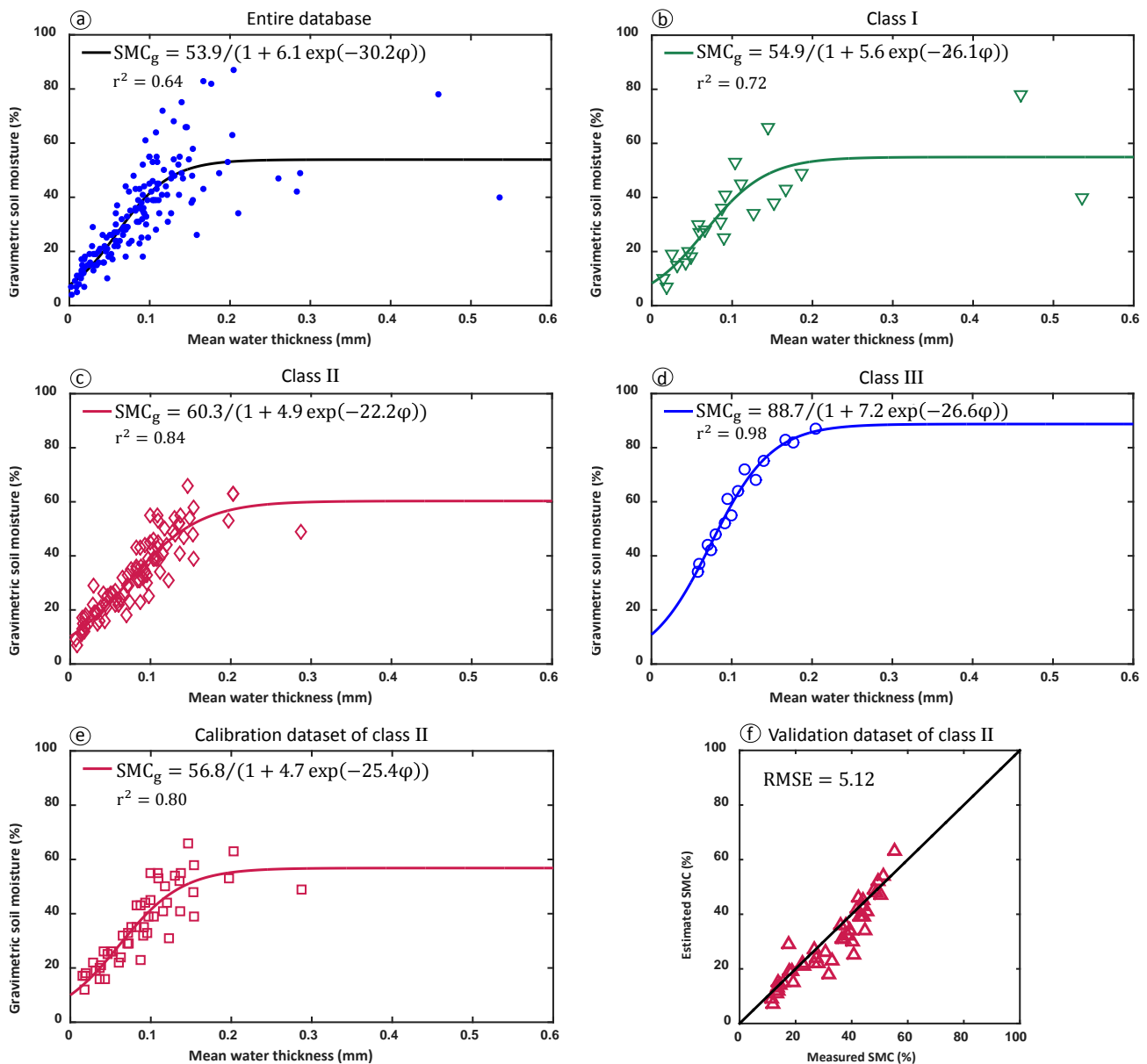


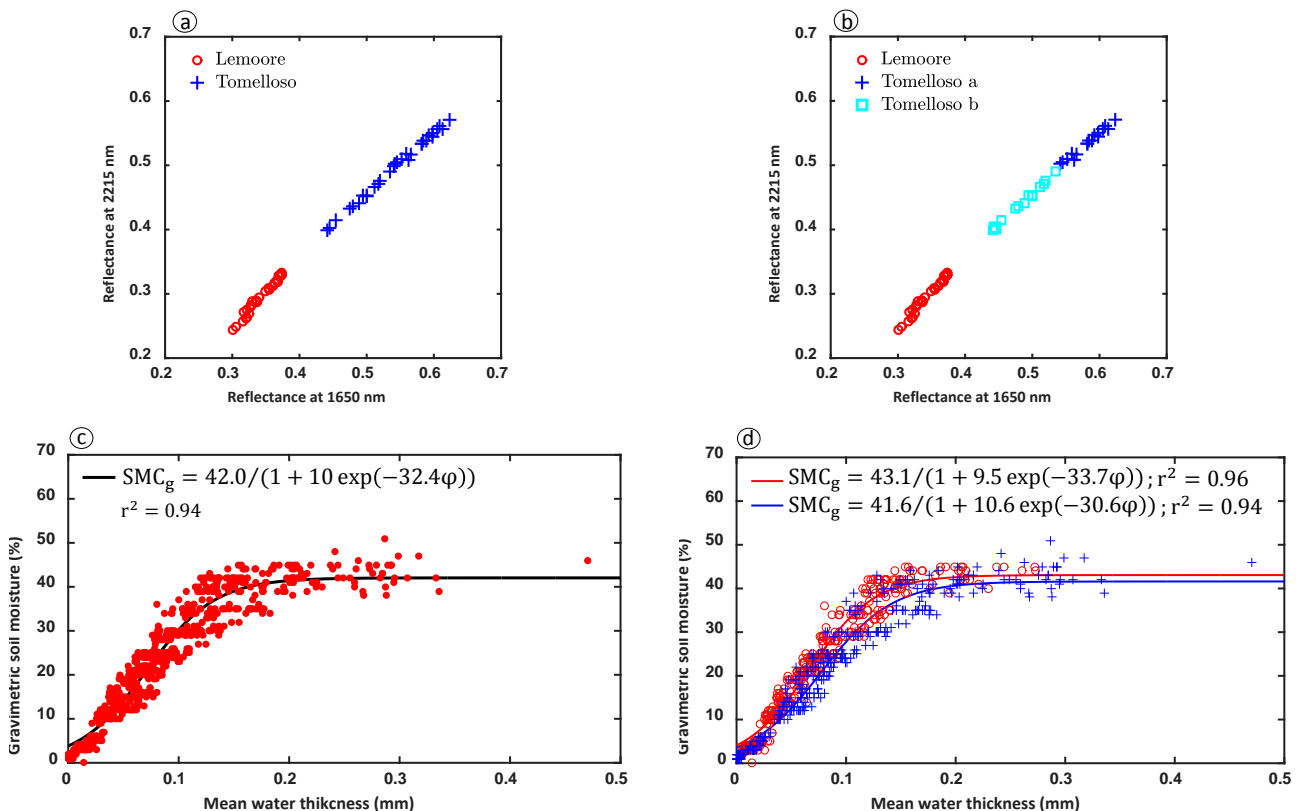
Fig. 14. Calibration phase for the different *a priori* classes of the Les08 dataset: (a) the thirty-two soils of the whole dataset, (b) the five soils of class I, (c) the sixteen soils of class II and (d) the three soils of class III. (e) Link between SMC and φ obtained with five soils of the class II and (f) estimated SMC thanks to the equation of calibration of (e) compared to measured SMC for the five soils of the validation dataset of class II.

441

442 Another classification method has been tested: [Lacerda et al \(2016\)](#) compare the reflectance of dry
 443 soils in Landsat-TM 5 band 5 (1650 nm) and band 7 (2215 nm). When one plots the second as a

444 function of the first, clayey soils and sandy soils are respectively located at the bottom and the top of
 445 the plot. The reflectance of sandy soils is often higher because they are often made of quartz (e.g.,
 446 Stoner and Baumgardner, 1981; Demattê, 2002; Lacerda et al., 2016). The Whit04 dataset that
 447 contains two different kinds of soils is well suited to test this method. Fig. 15a shows that the
 448 Tomelloso soils are located at the top of the plot and are scattered, while the Lemoore soils are located
 449 at the bottom and are concentrated. The calibration performed on the whole dataset globally led to a
 450 lower coefficient of determination ($r^2 = 0.94$) than that performed on the Lemoore and Tomelloso
 451 soils ($r^2 = 0.96$ and $r^2 = 0.94$, respectively) (Figs. 15c-d). Therefore, by using the same method of
 452 classification, we divided the Tomelloso soils into two subsets (Fig. 15b). The fit is slightly better
 453 with coefficients of determination higher than 0.95 and the two classes are clearly separated (Fig.
 454 15e). Once again the parameters of the sigmoid function, ψ and a , seem to be related to the
 455 mineralogy of the soils, which corroborates the result of Figs. 13a-b.

456



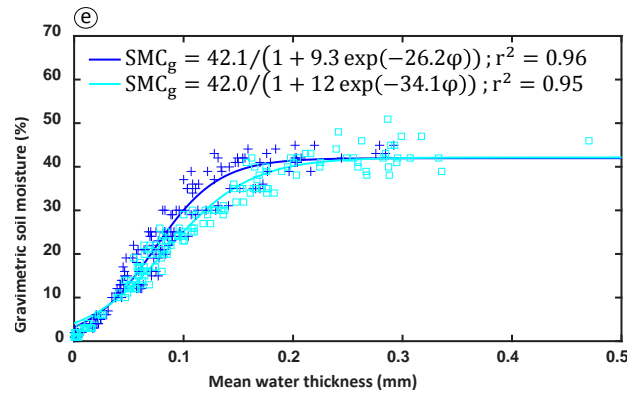


Fig. 15. Classification of the sixty soils of Whit04 after Lacerda et al. (2016). (a) Lemoore and Tomelloso separately and (b) Lemoore and Tomelloso when separated into two datasets. Calibration phase of the Whit04 dataset for (c) all the sample, (d) the thirty soil samples from Tomolleso and the thirty soil samples from Lemoore and (e) the thirty soil samples from Tomelloso soils divided into two datasets.

457

458 To validate this method of classification, a cross validation was performed on the Whit04 dataset
 459 by dividing the Lemoore soils into two subsets randomly chosen and equally sized, one for the
 460 calibration step (Fig. 16a) and one for the validation step (Fig. 16b). The soil moisture retrieval is very
 461 good (RMSE = 3.6%).

462

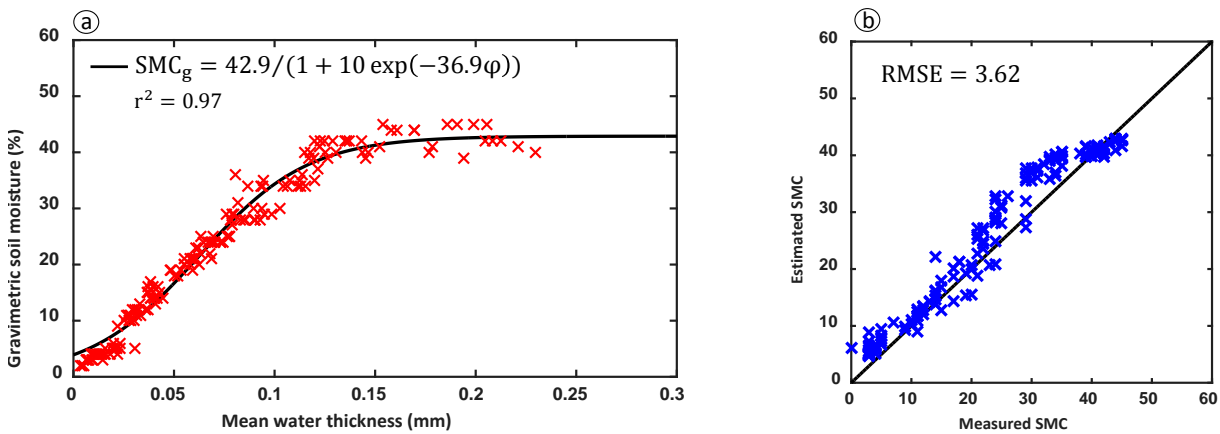


Fig. 16. (a) Calibration phase on eight soils from Lemoore and (b) prediction step on seven other soils of this same area.

463

464 We extended the study to the Lob02, Whit04, Les08 and Bab16 datasets all together. At this stage
 465 Liu02, Mar12 and Phil14 have been discarded due to different measurement protocols. Using the
 466 classification of Lacerda et al. (2016), three groups have been defined (Fig. 17a): group I contains a
 467 mixture of clayey and sandy soils, group II contains sandy soils and group III contains very sandy
 468 soils according to the Land Use and Management Brazilian Technical Classifications (LBTC). The r^2
 469 of groups I, II and III are respectively equal to 0.74, 0.83 and 0.92 when the r^2 of all the soils together

470 is 0.75 (Figs. 17b-e). So it will allow assessing the SMC of a soil of one of these groups with a good
 471 accuracy. Moreover, the coefficient K of the group III, which is made of sandy soils, is lower than that
 472 of the group I which is a mixture of sandy and clayey soils.

473

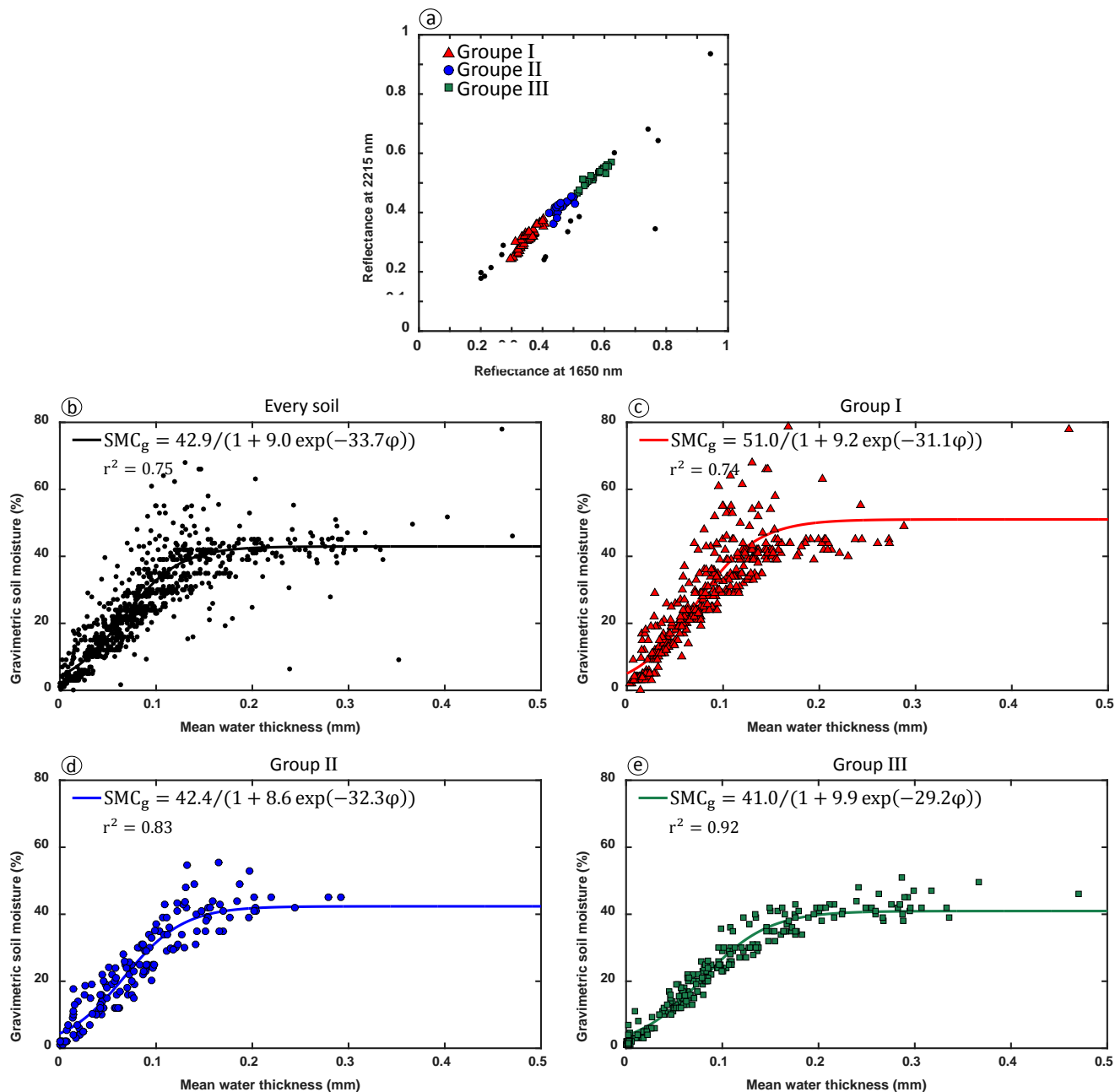


Fig. 17. (a) Lacerda classification method applied to ninety-seven soils of Lob02, Whit04, Les08 and Bab16, black dots are the unclassified samples. Calibration step on (b) all the soils of the datasets Lob02, Whit04, Les08 and Bab16, (c) fifty-three soils of group I, (d) twenty-two soils of group II and (e) the twenty-five soils of group III.

474

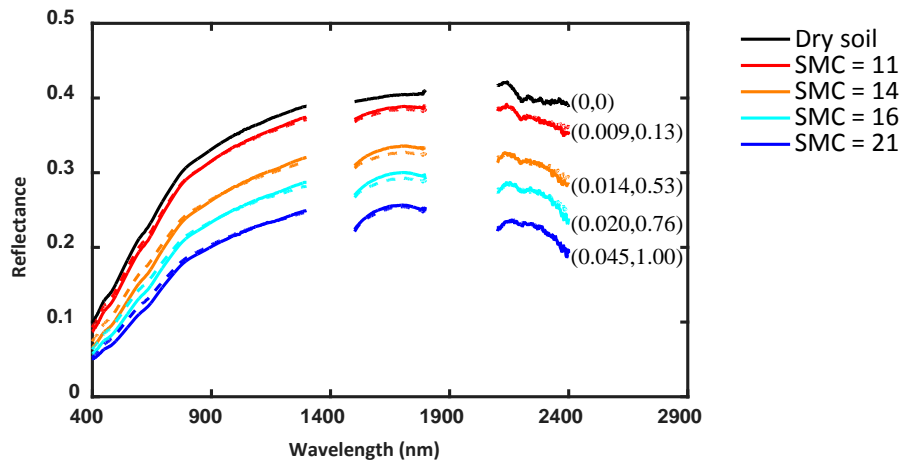
475 This method of classification seems to be adequate to build calibration equations that are strong
 476 enough to use MARMITforSMC globally. The next step is to use it outdoor, i.e., to see to what extent
 477 the atmospheric absorption bands affect the SMC retrieval.

478

479 3.3 MARMIT and MARMITforSMC without atmospheric absorption bands

480 In real conditions, part of the solar spectrum is not available because of atmospheric absorption
481 bands. We removed the two main bands located between 1300 nm and 1500 nm and between 1800 nm
482 and 2100 nm, and inverted MARMIT again. Fig. 18 shows a good fit of the data, which is not
483 surprising since Bach and Mauser (1994) came to the same conclusion with their model.

484

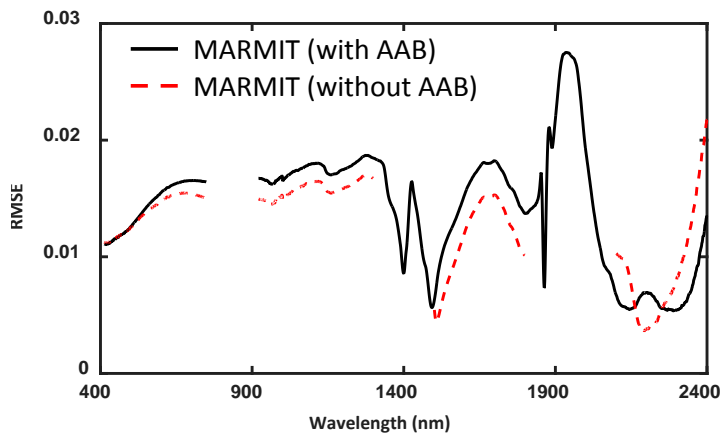


485 **Fig. 18.** Measured (solid line) and modeled (dashed line) reflectance spectra, excluding data in the main atmospheric
486 absorption bands of one soil at various levels of soil water content: soil from Ithaca in Phil14. The retrieved parameters
487 of the model are provided to the right of the curves (L, ϵ). L is in mm.

485

486 The RMSE obtained without the atmospheric absorption bands is even better (Fig. 19). The mean
487 water thickness estimated by inversion of MARMIT is very similar.

488



489 **Fig. 19.** RMSE obtained with MARMIT with and without reflectance data in the main atmospheric absorption bands
490 (AAB) for all the soils of all the database.

489

490 4. Comparison with other methods

491 In this section, the MARMITforSMC method described in [Section 3.2](#) is compared to other
 492 methods published in the literature for soil moisture content estimation. As they require calibration,
 493 we performed the calibration step and the assessment step on the same dataset as in [Sadeghi et al.](#)
 494 [\(2015\)](#).

495

496 4.2 Semi-empirical methods

497 Five spectral indices and two semi-empirical approaches, that are the Soil Moisture Gaussian
 498 Model (SMGM) ([Whiting et al., 2004](#)) and the relative absorption depth (RAD) through Continuum
 499 Removal method, were investigated. A spectral index is a combination of reflectances at two or more
 500 wavelengths: generally one chooses wavelengths where photons are not or little absorbed and
 501 wavelengths where, contrariwise, they are strongly absorbed. Most of the spectral indices listed in
 502 [Table 3](#) are typically used to determine soil water content. They perform quite well and are easy to
 503 use.

504

Index	Formula	Source
Normalized Soil Moisture Index (NSMI)	$\frac{R_{1800} - R_{2119}}{R_{1800} + R_{2119}}$	Haubrock et al. (2008)
Normalized Index of NSWIR domain for SMC estimation from Linear regression (NINSOL)	$\frac{R_{2076} - R_{2230}}{R_{2076} + R_{2230}}$	Fabre et al. (2015)
Normalized Index of NSWIR domain for SMC estimation from Non-linear regression (NINSON)	$\frac{R_{2122} - R_{2230}}{R_{2122} + R_{2230}}$	Oltra-Carrió et al. (2015)
Normalized Difference Water Index (NDWI)	$\frac{R_{860} - R_{1240}}{R_{860} + R_{1240}}$	Gao (1996)
Water Index SOIL (WISOIL)	$\frac{R_{1450}}{R_{1300}}$	Whalley et al. (1991)

Table 3. Some spectral indices found in the literature. Wavelengths are expressed in nm.

505

506 The SMGM and RAD methods are based on the continuum of the spectrum. Indeed, absorption
 507 features in the reflectance spectrum can be isolated by a mathematical function called apparent
 508 continuum ([Clark and Roush, 1984](#)). In the SMGM, [Whiting et al. \(2004\)](#) fit an inverted Gaussian
 509 function to the continuum and they calibrate the area below the curve to SMC. [Yin et al. \(2013\)](#)
 510 calculate the relative absorption depth as $R = 1 - R_b/R_c$ (where R_b is the normalized reflectance at

511 1940 nm and R_c the one at 1800 nm) and they regress it against SMC. In order to have a reliable
512 calibration, the results provided by these methods are compared to MARMITforSMC for datasets
513 containing more than five soil samples (Fig. 20). The worst results are obtained with the Liu02 and
514 Bab16 datasets, due to the nature of the soils described above. Let's now analyze the methods
515 individually:

516 1) The indices NSMI, NINSOL and NINSON which are known to perform well (Fabre et al., 2015)
517 provide the best results contrary to NDWI index which is mainly used for the detection of water in
518 vegetation (Gao, 1996; Khanna et al., 2007). NSMI, which performs best with Liu02, a dataset
519 containing oversaturated samples, seems to be the most appropriate index for saturated soils and
520 WISOIL also gives good results. But none of these both indices can be used in remote sensing
521 because one of the wavelength used is located in a broad atmospheric absorption band.

522 2) SMGM works well on Whit04 and Mar12 because the efficiency of this method depends on the
523 spectral shape of soil reflectance, which is very similar in these two datasets. The main
524 disadvantage of this method is that it is limited to soil below saturation with water content less than
525 0.32 g/g (Whiting et al., 2004).

526 3) The RAD method always leads to acceptable errors but never performs the best. It means that it
527 is robust but less efficient than NSMI, WISOIL and MARMITforSMC. Moreover, it has only been
528 tested on samples in laboratory conditions and it uses a wavelength located in one of the main
529 atmospheric absorption band (1940 nm).

530 4) MARMITforSMC performs very well and is the most robust method except for the Liu02
531 dataset for reasons already discussed.

532

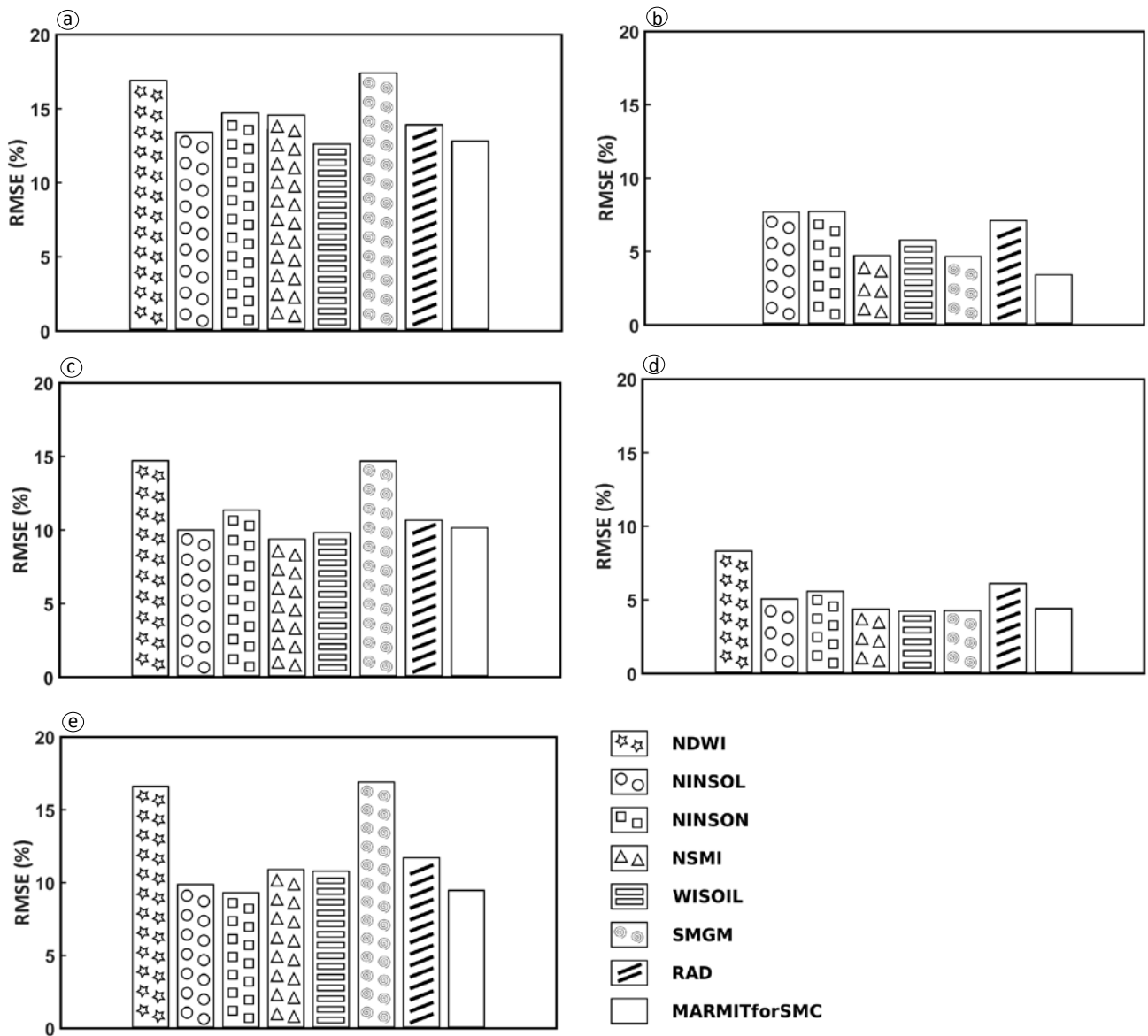


Fig. 20. Comparison of RMSE obtained with the spectral indices of Table 3, the SMGM and RAD methods, and MARMITforSMC using the datasets: (a) Liu02, (b) Whit04, (c) Les08, (d) Mar12 and (e) Bab16. NDWI cannot be applied to Whit04 because the reflectance at 860 nm is not available.

533

534 4.3 Physical models

535 4.3.1 The Sadeghi model

536 Sadeghi et al. (2015) developed a model based on the Kubelka-Munk theory. They provide two
 537 models, a complete one and a simplified one (Eq. (16)), which both link the SMC to the transformed
 538 reflectance of the wet soil (r), the dry soil (r_d), the saturated soil (r_s) and to the saturated SMC
 539 (SMCs):

540

$$SMC = \frac{r - r_d}{r_s - r_d} SMC_s \quad (16)$$

541

542 The transformed reflectance r is linked to soil reflectance R at 2210 nm (center of the Landsat-TM
543 and MODIS bands) by the relation $r = (1 - R)^2/2R$. [Sadeghi et al. \(2015\)](#) tested the efficiency of the
544 simplified model for SMC retrieval on two datasets: Lob02 and Whit04. For Lob02 they tested it soil-
545 by-soil and for Whit04 they separated the Lemoore soils from Tomelleso soils. They first performed a
546 calibration step: SMCs are measured and they obtain r_d and r_s thanks to a least square optimization.
547 Then they used this calibration equation to assess SMC. [Table 4](#) provides the RMSE of SMC retrieved
548 using the Sadeghi model and using MARMITforSMC.

549

Dataset	Soil	RMSE (%)	
		Sadeghi	MARMITforSMC
Lob02	Andisol	3.6	2.4
	Entisol	1.2	2.4
	Aridisol	0.5	1.1
	Mollisol	3.0	2.8
Whit04	Lemoore	6.7	2.7
	Tomelloso	7.7	3.3

Table 4. Comparison of SMC assessment with MARMIT compared to the one with the Sadeghi model. In bold the best results.

550

551 MARMITforSMC performs much better than the Sadeghi model for the Whit04 dataset while the
552 results are similar for the Lob02 dataset, depending on the soil. The RMSE are divided by more than
553 two because, in the calibration phase of the Sadeghi model, only one transformed reflectance
554 spectrum of dry and wet soil can be obtained by inversion even if different soils are studied. In
555 MARMIT the reflectance spectrum of the dry soil is used for each soil.

556

557 4.3.2 The Bach model

558 As mentioned in [Section 2.1](#), MARMIT derives from the Bach model ([Eq. \(5\)](#)). [Bach \(1995\)](#) also
559 performs a calibration of her model but she relates SMC with L using a linear regression. We decided
560 to apply the same calibration phase as in MARMITforSMC and to link φ and SMC with a sigmoid
561 function. The entire dataset Whit04 and the three classes of Les08 have been compared. MARMIT
562 leads to a better RMSE ([Table 5](#)), even if the Bach model better fits the measured reflectance spectra
563 ([Fig. 6](#)) due to an adapted water absorption coefficient.

Dataset		RMSE (%)	
		Bach	MARMITforSMC
Whit04		4.8	3.4
Les08	Whole dataset	7.1	6.7
	Class I	7.0	6.7
	Class II	4.8	4.3
	Class III	2.9	2.1

Table 5. Comparison between MARMIT and the Bach model. In bold the best RMSE.

565

566 5. Conclusion

567 A simple physically-based model called MARMIT was developed and used for SMC retrieval on
568 seven independent datasets gathering 217 soil samples collected in China, France, Spain, Tunisia and
569 the U.S.A. The model estimates SMC in three key steps which constitutes the MARMITforSMC
570 method: (1) inversion, (2) calibration, and (3) (cross-)validation. Step (1) works better for low SMC
571 values. Sometimes it is difficult to fit the reflectance in the visible probably because some phenomena
572 are not taken into account: for instance, it is likely that the soil particles and the water film mix as
573 suggested by [Philpot \(2010\)](#). This leads to an overestimation of the reflectance outside the water
574 absorption bands and an underestimation in the water absorption bands. Despite this issue, step (2)
575 explains very well the evolution of SMC with φ when soils are considered individually ($r^2 \geq 0.95$).
576 The variation of soil moisture content as a function of the mean water thickness is well described by a
577 sigmoid function, some parameters of which are related to soil chemical and physical properties. The
578 parameter K (maximum value of the function) seems to be linked with the SMC at saturation; a (the
579 place of the curve on the x-axis) and ψ (the slope between the two horizontal asymptotes) may be
580 related to mineralogy. Unfortunately, we lack metadata to support this hypothesis. As the goal of the
581 method is to infer the SMC using remote sensing data regardless of the soil type, a soil-by-soil
582 calibration is not desirable. We successfully grouped the soils together into general classes to infer
583 accurate global calibration equations. The most operational way of classification proposed by [Lacerda
584 et al. \(2016\)](#) has been successfully tested on the thirty Lemoore soils of the Whit04 dataset ($RMSE =$
585 3.62%) and more generally on the soils of the datasets Lob02, Whit04, Les08 and Bab16 together.

586 Indeed, we found three groups with coefficients of determination of the relationship between SMC
587 and φ greater than 0.74. Finally, MARMITforSMC has been compared to existing methods for SMC
588 retrieval: the method performs as well or better than other methods, especially the one relying on the
589 Bach model. Moreover, we proved that SMC could be retrieved with the same accuracy as TDR
590 measurements thanks to an appropriate classification (RMSE \sim 3%). The new method clearly led to
591 an improvement in the SMC retrieval. The main advantage of this model is that it is easy to
592 understand and fast to compute, and there is room for progress. The drawback of MARMITforSMC is
593 that it requires a calibration step, which is soil dependent, and the reflectance spectrum of the dry soil.
594 The first issue can be overcome with a soil classification based on spectral signatures and the second
595 one by multi-data imagery. We also showed that MARMIT was not suitable for oversaturated soils in
596 water. The model may be improved by taking into account specular reflectance. The measurement
597 protocol, e.g., water distribution within the sample, probably influences the results of
598 MARMITforSMC given that the SMC in the sample is variable vertically and horizontally. Future
599 research in SMC retrieval using MARMIT with soils of known textural and mineralogical properties
600 will help extend and improve the model for porosity or grain size.

601

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