

1 **Combining frequency domain reflectometry and visible and near infrared**  
2 **spectroscopy for assessment of soil bulk density**

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8  
9 **Abstract**

10 This paper introduces a new approach for the assessment of soil bulk density (BD), which  
11 relies on an existed model to predict BD as a function of a visible and near infrared  
12 spectroscopy (vis-NIRS) measured gravimetric moisture content ( $\omega$ ) and a frequency domain  
13 reflectometry (FDR) measured volumetric moisture content ( $\theta_v$ ). A total of 1013 soil samples  
14 collected from England and Wales, from 32 arable and grassland fields with different soil  
15 types were measured with a vis-NIR spectrophotometer (LabSpec®Pro Near Infrared  
16 Analyzer, Analytical Spectral Devices, Inc, USA) after *in situ* measurement with a  
17 ThetaProbe FDR (Delta-T Device Ltd). Two calibration methods of the vis-NIRS were  
18 tested, namely, partial least squares regression (PLSR) and artificial neural network (ANN).  
19 ThetaProbe calibration was performed with traditional methods and ANN. ANN analyses  
20 were based on a single input or multiple input variables (data fusion). During ANN - data  
21 fusion analysis, vis-NIRS spectra and ThetaProbe output voltage (V) were fused in one  
22 matrix with or without laboratory measured texture fractions and organic matter content  
23 (OM). For the vis-NIRS and ThetaProbe traditional calibration, samples were divided into  
24 calibration (75 %) and prediction (25 %) sets, whereas for the ANN analysis these were  
25 divided into calibration (65%), test (10%) and independent validation (25%) sets. Results

26 proved that high measurement accuracy can be obtained for  $\omega$  and  $\theta_v$  with PLSR and the best  
27 performing traditional calibration method of the ThetaProbe with  $R^2$  values of 0.91 and 0.97,  
28 and root mean square error of prediction (RMSEp) of  $0.027 \text{ g g}^{-1}$  and  $0.019 \text{ cm}^3 \text{ cm}^{-3}$ ,  
29 respectively. However, the ANN – data fusion resulted in improved accuracy ( $R^2 = 0.98$  and  
30  $\text{RMSEp} = 0.014 \text{ g g}^{-1}$  and  $0.015 \text{ cm}^3 \text{ cm}^{-3}$ , respectively). This data fusion approach led to the  
31 best accuracy for BD assessment when vis-NIRS spectra and ThetaProbe V only were used as  
32 input data ( $R^2 = 0.81$  and  $\text{RMSEp} = 0.095 \text{ g cm}^{-3}$ ). It can be concluded that BD can be  
33 measured by combining the vis-NIRS and FDR techniques based on ANN-data fusion  
34 approach.

35

36 Keywords: Bulk density, multi-sensor, data fusion, vis-NIR spectroscopy, FDR.

37

## 38 **1. Introduction**

39 Forest, arable and grasslands are important natural resources, which have been subjected to  
40 artificial and natural compression stresses through the ages. Heavy agriculture machinery,  
41 intensive use of the arable lands and livestock impact on grasslands during the wet soil  
42 conditions, are among the major factors causing compression stresses, which lead to soil  
43 compaction (Vrindts et al., 2005). Soil compaction is normally associated with damage of the  
44 soil structure, deterioration of physical and hydraulic properties and creation of unfavourable  
45 conditions for plant root system. Compacted soils demand large amount of fertilisers, in order  
46 to substitute the small volume available for plant roots, which might cause contamination  
47 hazardous of the ground water by the deep percolation or the run off to the surface water  
48 (Soane and van Ouwerkerk, 1995). Highly compacted soils can be considerably of low  
49 productivity and require more mechanical power for soil preparations. Among other  
50 parameters used to assess soil compaction, bulk density (BD) that is the closer packing of

51 solid particles or the reduction in porosity is a widely used parameter (Grossman, 1981;  
52 Bardy, 1984; Singh et al., 1992; Wuest et al., 2009). However, BD might be considered as a  
53 sing of soil compaction, as it does not necessarily reflect soil functioning (e.g. air and water  
54 movement) (Quraishi and Mouazen, 2013a). Other parameters e.g. saturated hydraulic  
55 conductivity and infiltration rate are more closely related to soil compaction (Fleige and  
56 Horn, 2000), as compared to BD. However, in comparison with the latter parameters,  
57 assessment of BD with a portable system is possible (Quraishi and Mouazen, 2013a) and  
58 enables faster, easier and more cost effective data acquisition, which is particularly useful for  
59 precision agriculture applications.

60 The most common traditional method for BD measurement is the core sampling method (e.g.  
61 Kopecki ring), which is laborious, time consuming, expensive and difficult to conduct under  
62 dry soil conditions (Quraishi and Mouazen, 2013b). This is the reason why penetrometers to  
63 measure soil penetration resistance, known as cone index is widely used to map the variation  
64 in soil compaction with depth (Sun et al., 2011). However, Mouazen and Ramon (2006)  
65 explained that penetration resistance is simultaneously affected by moisture content, texture,  
66 BD and organic matter content (OM). Therefore, a new method to measure BD is required  
67 that should be fast, easy, cost effective and do not need an expert operator.

68 For years, visible and near infrared spectroscopy (vis-NIRS) has provided a proven and  
69 versatile analytical method for soil analyses (Viscarra Rossel & McBratney, 1998; Shepherd  
70 & Walsh, 2002; Clark et al, 2005; Mouazen et al, 2010; Stenberg et al., 2010). It is fast  
71 measurement technique, non-destructive and cost effective (Mouazen et al., 2005). It was  
72 successfully used to measure gravimetric moisture content ( $\omega$ ) under laboratory non-mobile  
73 measurement conditions (Dalal and Henry, 1986; Slaughter et al., 2001; Lobell and Anser,  
74 2002; Mouazen et al., 2006a) and on-line mobile conditions (Mouazen et al., 2005). These

75 successful applications were attributed to the strong influence of O-H bond on vis-NIR  
76 spectra of soils (Kuang et al., 2012; Stenberg et al., 2010).

77 The measurement of dielectric constant ( $K$ ) based on frequency domain reflectometry (FDR)  
78 is a popular technique for the measurement of soil volumetric moisture content ( $\theta_v$ ) (Topp et  
79 al., 1980; Miller and Gaskin, 1997; Robinson et al., 1999). This is due to the fact that  $K$  of the  
80 water ( $\sim 80$ ) is significantly greater than that of the dry soil matrix materials ( $\sim 4$ ) and of the  
81 air ( $\sim 1$ ). ThetaProbe (Delta-T Devices Ltd., 1999) was reported to be capable to measure soil  
82  $\theta_v$  with  $\pm 0.01 \text{ m}^3 \text{ m}^{-3}$  accuracy after a single two-point gravimetric calibration, although,  
83  $\pm 0.05 \text{ m}^3 \text{ m}^{-3}$  accuracy can be achieved when generalised calibration by the manufacturer is  
84 applied (Foley and Harris, 2007; Kaleita et al., 2005; Jones et al., 2002; Walker et al., 2004).

85 Multiple sensor and data fusion is being introduced as a new concept in proximal soil sensing  
86 (Kuang et al., 2012). Data fusion is an important tool that may improve the performance of a  
87 detecting system while various integrated sensors are available (Mahmood et al., 2009).

88 Despite the fact that this is a new concept, several studies were reported for non-mobile  
89 (Hummel et al., 2004; Quraishi and Mouazen, 2013b) and mobile (Glancey et al., 1989;  
90 Mouazen et al., 2003; Adamchuk et al., 2004; Mouazen et al., 2005; Mouazen and Ramon,  
91 2006; Naderi-Boldaji et al., 2012; Quraishi and Mouazen, 2013c) measurement conditions.

92 Quraishi and Mouazen (2013b) reported a data fusion approach of BD assessment, based on  
93 the fusion of data on  $\omega$ , OM and clay content (C), measured with a vis-NIR  
94 spectrophotometer and penetration resistance measured with a penetrometer. However, a  
95 large number of variables e.g.  $\omega$ , OM, C and penetration resistance is needed as input for the  
96 artificial neural network (ANN) to predict BD is required. The accumulated error of vis-NIR  
97 measurement of  $\omega$ , OM and C would sum up to a considerable error of BD assessment.

98 Therefore, a simpler approach is needed that is based on a fusion of fewer input variables  
99 (e.g.  $\omega$  and  $\theta_v$ ), where error in BD assessment is small.

100 The aim of the paper is to introduce a new approach for BD assessment to be adopted for  
101 precision agriculture applications, which is based on a multi-sensor and data fusion approach.  
102 It relies on combining the vis-NIRS measurement of  $\omega$  and ThetaProbe measurement of  $\theta_v$ ,  
103 which are substituted into an existed model to predict BD.

104

## 105 **2. Materials and methods**

### 106 *2.1. Experimental sites and soil samples*

107 A total of 1013 undisturbed soil samples were collected, at the same time of the field  
108 measurement, from 32 fields in seven locations in England e.g. Silsoe and Wilstead in  
109 Bedfordshire, Haversham and Gayhurst in Buckinghamshire, Flawborough in  
110 Nottinghamshire, Nafferton and Morpeth in Northumberland and from one location in Wales  
111 e.g. Brecon. They have been collected from the top layer of 10-20 cm between May, 2011  
112 and December, 2012. Detailed information about these fields is shown in Table 1. These  
113 fields were of a wide range of soil texture (Fig. 1), moisture content, OM and BD and were  
114 under different land use (Tables 1 and 2). This wide variability is advantage to allow testing  
115 the applicability of the new measurement system of BD under different field conditions. Soil  
116 cores were collected by a rigid ploy vinyl chloride (PVC) cylinder of 60 mm height and 50  
117 mm in diameter, and were transferred to the laboratory for further analysis. All soil cores  
118 were kept in the PVC cylinders sealed in plastic pages to prevent moisture losing. They  
119 stored at 4 °C from the time of sampling until the time of analysis.

120

### 121 *2.2. Laboratory analysis*

122 Soil BD,  $\theta_v$ ,  $\omega$  for all 1013 samples were measured by oven drying of samples at 105°C for  
123 24 h (British Standards, 2007). Particle size distribution (PSD) and OM were measured for  
124 average field samples. The PSD was measured by sieving and sedimentation method (British

125 Standards, 1998). Soil OM was measured with a TrusSpecCNS spectrometer (LECO  
126 Corporation, St. Joseph, MI, USA), using the Dumas combustion method (British Standards,  
127 2000). Results of laboratory analyses are shown in Tables 1 and 2.

128

### 129 ***2.3. Soil bulk density estimation***

130 The following relationship exists between BD,  $\omega$  and  $\theta_v$  (Wijaya et al., 2004):

131

$$132 \quad BD = \theta_v / \omega \quad (1)$$

133 Where: BD is the soil bulk density in  $\text{g cm}^{-3}$ ,  $\theta_v$  is the volumetric moisture content in  $\text{cm}^3 \text{ cm}^{-3}$   
134 and  $\omega$  is the gravimetric moisture content in  $\text{g g}^{-1}$ .

135 The hypothesis of this study is that by substituting  $\theta_v$  measured with a ThetaProbe and  $\omega$   
136 measured with a vis-NIR spectrophotometer into Eqn (1), BD can be derived with acceptable  
137 accuracy as compared to the oven drying method of soil samples at 105 °C for 24 h. This  
138 hypothesis will be tested in this study.

139

### 140 ***2.4. ThetaProbe and visible and near infrared spectroscopy***

141 A ThetaProbe and a vis-NIR spectrophotometer were used to measure  $\theta_v$  and  $\omega$ , respectively.

142 A detailed description of the measurement is provided in the following subsections.

143

#### 144 **2.4.1. ThetaProbe description**

145 ThetaProbe (Delta-T Devices Ltd., 1999) is the commercial name of dielectric probe to  
146 measure  $\theta_v$ . It has been developed jointly by the Macaulay Land Use Research Institute,  
147 Scotland and Delta-T Devices Ltd, Cambridge. ThetaProbe consists of waterproof housing,  
148 which contains electronic circuit attached to it at one end, and four parallel stainless steel rods  
149 of 60 mm long and 3 mm in diameter, to be inserted into the soil and at the other end

150 input/output cable (Fig. 2). The electronic circuit generates and emits electromagnetic signal  
151 of sinusoidal shape, which is applied to an internal transmission line to the array of four rods.  
152 The impedance of this array varies according to the impedance of the soil, which has two  
153 components, namely, the apparent dielectric constant ( $K$ ) and the ionic conductivity. A 100  
154 MHz of frequency was chosen in order to minimise the effect of ionic conductivity, so that  
155 changes in the transmission line impedance dependent almost solely on the soil's apparent  $K$ .  
156 Water content determines  $K$  of the soil, as  $K$  of the water (~81) is much higher than  $K$  of the  
157 soil (3 to 5) and that of the air (1). The traveling electromagnetic wave through the soil mass  
158 will cause a voltage standing wave to be set up from the interference of the emitted signal and  
159 its reflected component. By measuring this voltage amplitude,  $K$  of the soil can be obtained  
160 and thus  $\theta_v$ . More details can be found in Gaskin in Miler (1996) and Miller and Gaskin  
161 (1997). Kaleita et al. (2005) studied the effect of soil temperature on laboratory calibration of  
162 ThetaProbe, and found insignificantly differences in the accuracy for a temperature range of  
163 10 to 40 °C. Insignificant effect of soil salinity in the range of 250 - 2000 mS m<sup>-1</sup> was  
164 confirmed by the ThetaProbe manufacturer (Delta-T Devices Ltd., 1999).

165

#### 166 **2.4.2. ThetaProbe calibration and validation**

167 Three ThetaProbe readings were recorded *in situ* from the same spot (e.g. 50 cm in diameter),  
168 where the soil core was collected. Additional reading was also recorded from the soil core  
169 itself. These four readings were averaged in one final reading. In this study, five methods for  
170 the calibration of ThetaProbe were tested, namely, manufacturer (M), specific soil calibration  
171 (SSC), general formula (GF) (Topp et al. 1980), and ThetaProbe output voltage (OV) and  
172 ANN. The input for all calibration was the readout of the ThetaProbe only. In the following  
173 subsections, the first four methods are explained, whereas, for simplicity, ANN is explained  
174 in a later section.

175

176 **2.4.2.1. Manufacturer calibration method (M)**

177 The general calibration by the manufacturer of the device is a pre-set programme at  
178 ThetaProbe digital moisture meter type (HH2), which provides instant readout of  $\theta_v$  and also  
179  $V$ . It comprises two calibration options for mineral and organic soils (Delta-T Devices Ltd.,  
180 1999). It is based on the following third order relationship between  $K$  and  $V$ :

181

$$\sqrt{K} = 1.07 + 6.4V - 6.4V^2 + 4.7V^3 \quad (2)$$

182

183 Where  $\sqrt{K}$  is the square root of the dielectric constant and  $V$  is the output voltage reading of  
184 the ThetaProbe.

185 By substituting  $\sqrt{K}$  into the following equations,  $\theta_v$  can be calculated for mineral and organic  
186 soils, respectively:

187

$$\theta_v = \frac{\sqrt{k}-1.6}{8.4} \quad (3)$$

$$\theta_v = \frac{\sqrt{k}-1.3}{7.7} \quad (4)$$

188

189 **2.4.2.2. Specific soil calibration method (SSC)**

190 This method relies on Eqn. (1), but is used for specific soil types. To calculate  $\theta_v$  for a  
191 specific soil, the following linear relationship between  $\sqrt{K}$  and  $\theta_v$  was established (Delta-T  
192 Devices Ltd., 1999):

193

$$\theta_v = \frac{\sqrt{K}-a_0}{a_1} \quad (5)$$

194



195 Where  $a_1$  and  $a_0$  are coefficients for wet and dry soil sample, respectively.  $a_0$  is considered  
196 equal to  $\sqrt{K_0}$  (Gaskin and Miller, 1996). However,  $a_1$  is calculated from the following  
197 equation:

$$a_1 = \frac{\sqrt{K_1} - \sqrt{K_0}}{\theta_{vt}} \quad (6)$$

198  
199  
200  $\sqrt{K_1}$  is the square root of the dielectric constant of the wet undisturbed soil sample,  $\sqrt{K_0}$  is  
201 the square root of the dielectric constant of the dried undisturbed soil sample, both  $\sqrt{K_1}$   
202 and  $\sqrt{K_0}$  were measured using Eqn. (2),  $\theta_{vt}$  is measured volumetric moisture content by oven  
203 drying of samples for 105 °C for 24 h.

204

#### 205 **2.4.2.3. General formula calibration method (GF)**

206 This method relies on the concept that  $K$  can be measured from the standing voltage of the  
207 soil matrix and thus indicates  $\theta_v$ . Topp et al., (1980) established the universal equation to  
208 express the relation between  $\theta_v$  and  $K$  of many soil types, collected from all over the world,  
209 which is written as follows:

210

$$\theta_v = -0.053 + 0.0292K - 0.00055K^2 + 0.0000043K^3 \quad (7)$$

211

212 The  $K$  value is derived based on average measured  $V$ , which is substituted into Eqn. 7. to  
213 calculate  $\theta_v$ .

214

#### 215 **2.4.2.4. Output voltage calibration method (OV)**

216 In this method a direct relationship between  $V$  and  $\theta_v$  was established based on *in situ*  
217 measurement of ThetaProbe of soils collected in the current study. The average spot

218 ThetaProbe output readings of 1013 samples were divided into two sets, namely, calibration  
219 (75%) and independent validation set (25%). The former was used to generate the  
220 relationship between  $\theta_v$  and  $V$ , whereas the latter was used to validate the calibration  
221 equation developed.

222

## 223 **2.5. Visible and near infrared spectrophotometer calibration and validation**

224 The fresh, remoulded soil samples were scanned in the laboratory in three replicates, by a  
225 LabSpec vis-NIR portable spectrophotometer (LabSpec Pro Near Infrared Analyzer,  
226 Analytical Spectral Devices, Inc, USA) (ASDi). The diffuse reflected light from the top 2-3  
227 mm layer of 117.75 cm<sup>3</sup> cylindrical samples was collected. The spectrophotometer has one Si  
228 array (350 – 1000 nm) and two Peltier cooled InGaAs detectors (1000 –1800 nm and 1800 –  
229 2500 nm). Spectra sampling interval of the instrument was 1 nm across the entire spectra  
230 range. However, the spectral resolution was 3 nm at 700 nm and 10 nm at 1400 and 2100 nm.  
231 A high intensity probe with a light source built in of a quartz-halogen bulb of 3000 K° light  
232 was used. The detection fibres were gathered in the high intensity probe enclosing 35° angle.  
233 Before scanning, only large plant residues, debris and stones were removed from the fresh  
234 samples (Mouazen et al., 2005). Different amounts of non-sieved soil according to different  
235 textures were packed in Petri dishes of a 1.0 cm height by 3.6 cm in diameter. Soil in a Petri  
236 dish was mixed properly and a gentle pressure was applied on the surface with a spatula to  
237 generate levelled and smooth surface to ensure a maximum diffuse reflection and thus a good  
238 signal-to-noise ratio (Mouazen et al., 2007). Before the soil samples were scanned and at  
239 intervals of 30 min, a white reference Spectralon disc was scanned. Three readings were  
240 collected from each soil sample and these were averaged in one spectrum to be used for  
241 spectra pre-treatment and model establishment.

242

### 243 **2.5.1. Spectra pre-treatment and establishment of calibration model**

244 Spectra pre-treatment aimed to reduce spurious peaks that do not contain physical or  
245 chemical information and to correct physical scatter effects. Soil spectra range was first  
246 reduced to 500– 2200 nm, to eliminate noise at both edges and to enhance calibration  
247 accuracy for  $\omega$  measurement (Mouazen et al., 2005). After noise cut, spectra were reduced by  
248 averaging 10 successive wavelengths. Maximum normalisation was followed, which is  
249 typically used to get all data to approximately the same scale, or to get a more even  
250 distribution of the variances and the average values. The maximum normalisation is a  
251 normalisation that “polarizes” the spectra. The peaks of all spectra with positive values were  
252 scaled to + 1, while spectra with negative values were scaled to – 1. Since soil spectra have  
253 maximum positive values, the peaks of these spectra were scaled to + 1 (Mouazen et al.,  
254 2005). The maximum normalisation led to better results for  $\omega$  measurement, compared to  
255 other pre-treatment options tested. Spectra were then subjected to Savitzky–Golay first  
256 derivation transformation (Martens and Naes, 1989). This method enables to compute the  
257 first or higher order derivatives, including a smoothing factor, which determines how many  
258 adjacent variables will be used to estimate the polynomial approximation used for  
259 derivatives. A second order polynomial approximation was selected. A 2:2 smoothing was  
260 carried out after the first derivative to decrease noise from the measured spectra. All pre-  
261 treatment steps were carried out using Unscrambler 7.8 software (Camo Inc.; Oslo, Norway).  
262 The entire 1013 soil spectra were divided into calibration (75%) and independent validation  
263 (25%) sets. Partial least squares regression (PLSR) was implemented using the calibration set  
264 to relate the variation in one response variable (e.g.  $\omega$ ) to the variation in multi-spectra  
265 wavelengths, using Unscrambler 7.8 software (Camo Inc.; Oslo, Norway). It is a bilinear  
266 modelling method where information in the original x data is projected onto a small number  
267 of underlying (“latent”) variables called PLS components. The y data are actively used in

268 estimating the “latent” variables to ensure that the first components are those that are most  
269 relevant for predicting the y variables. Interpretation of the relationship between x data and y  
270 data is then simplified as this relationship is concentrated on the smallest possible number of  
271 components. More detailed information about the PLSR can be found in Martens and Naes  
272 (1989).

273 To evaluate model accuracy for the measurement of  $\omega$ , the root mean square error of  
274 prediction ( $RMSEP$ ) of the independent validation set was considered. The coefficient of  
275 determination ( $R^2$ ) and residual prediction deviation (RPD), which is the ratio of standard  
276 deviation (SD) values of the laboratory measured  $\omega$  divided by  $RMSEP$  of the independent  
277 validation set were also considered to evaluate the performance of calibration models  
278 (Mouazen et al., 2010). Mouazen et al. (2006b) proposed the following classes of the RPD  
279 values: an RPD value below 1.5 indicates poor model predictions and that such a value could  
280 not be useful; an RPD value between 1.5 and 2.0 indicates a possibility of distinguishing  
281 between large and small values, while a value between 2.0 and 2.5 makes approximate  
282 quantitative predictions possible. For RPD values between 2.5 and 3.0 and above 3.0, the  
283 prediction is classified as good and excellent, respectively. This classification system of RPD  
284 was adopted in this study. Generally, a good model performance would have high  $R^2$  and  
285 RPD values, and a small value of  $RMSEP$ .

286

## 287 **2.6. Data fusion and modelling**

288 Methods adopted in sections 2.2. and 2.3. for the measurement of  $\theta_v$  and  $\omega$ , respectively,  
289 were based solely on output signal of ThetaProbe or vis-NIRS, respectively. In this section,  
290 the measurement of  $\theta_v$  and  $\omega$  is based on fusion of output data from both sensing techniques  
291 ( $V$  and spectra) with or without data obtained from laboratory analysis on sand (S in %), silt  
292 (SL in %), C in % and OM in %. However, in order to compare with other data fusion

293 models, input data of  $V$  or soil spectra were used for the measurement of  $\theta_v$  and  $\omega$ ,  
294 respectively.

295 One of the tools available for data fusion is the ANN. Neural networks are simplified models  
296 of the biological structure of human brains (Günaydin, 2009). There are three main layers in  
297 the ANN structure, namely, a set of input nodes, one or more layers of hidden nodes and a set  
298 of output nodes. In this study, different number of nodes was used in each layer depending on  
299 the input data used (Fig. 3). For instance, the number of nodes of the hidden layer for  $\theta_v$   
300 based on  $V$  only was two layers (Table 3). Seven ANN analyses were performed to develop  
301 different models, according to the different input variables used (Table 3). The output layers  
302 for different combinations were  $\theta_v$  or  $\omega$ , or both. All the modelling cases were developed  
303 with Statistica software (StatSoft, USA, 2011). The powerful second order Broyden–  
304 Fletcher–Goldfarb–Shanno (BFGS) training algorithms, with different transfer functions used  
305 for hidden and output layers were used, as detailed in Table 3. The transfer functions  
306 included hyperbolic tangent (Tanh), logarithmic (Log) and exponential (Exp). The number of  
307 neurons in the hidden layer is established by training several networks with different number  
308 of hidden neurons, and comparing the predicted with measured values. In this study, a hidden  
309 layer with five neurons showed the best results. Data for the entire 1013 soil samples were  
310 divided into training set (65%), test set (10%) and independent validation set (25%). All the  
311 texture classes were included in the three sets so that the resulted models are valid for all  
312 textures.

313 The measured values of  $\omega$  and  $\theta_v$  obtained, respectively, based either on the traditional  
314 calibration of the vis-NIRS and ThetaProbe or on the ANN analyses were used to predict BD  
315 using Eqn. (1). The performance of the developed models was evaluated by means of  $R^2$  and  
316 RMSEp.

317

### 318 3. Results and discussion

319

#### 320 3.1. Accuracy of ThetaProbe measurement for volumetric moisture content

321 Table 4 shows the results of the measurement accuracy of  $\theta_v$  with the ThetaProbe against the  
322 oven drying method using M, SSC, GF, OV and ANN calibration models with one input  
323 parameter (e.g. output voltage  $V$ ). Results suggest that the ThetaProbe is capable to measure  
324  $\theta_v$  with high accuracy even with the M calibration method, without the need for additional  
325 calibration. However, slight differences can be observed between these methods. With the M  
326 method, the measured values of  $\theta_v$  overestimate the oven drying measured values. Working  
327 with M method, Robinson et al. (1999) and Kaleita et al. (2005) observed similar  
328 overestimation for a group of soil samples across a full range of moisture content. Both  
329 research groups indicated that the accuracy of the ThetaProbe declined with moisture content,  
330 which is a similar trend observed in the current study. The scatter plot of the ThetaProbe-M  
331 predicted versus oven drying measured  $\theta_v$  illustrates intercept with x axis with a value of  
332  $1.12 \text{ cm}^3 \text{ cm}^{-3}$ , indicating overestimation of the M model (Fig. 4). The SSC calibration  
333 method performs as equal as that of the M method. However, the GF calibration method  
334 provide an improved measurement accuracy ( $R^2 = 0.96$  and  $\text{RMSEp} = 0.020 \text{ cm}^3 \text{ cm}^{-3}$ ) (Table  
335 4). The RMSEp obtained with these three methods (e.g. M, SSC and GF) is still larger than  
336  $0.01 \text{ m}^3 \text{ m}^{-3}$ , which contradicts the instruction provided by the ThetaProbe's manufacturer.  
337 The OV calibration method leads to further improvement ( $R^2 = 0.97$  and  $\text{RMSEp} = 0.019 \text{ cm}^3$   
338  $\text{cm}^{-3}$ ), as compared to the M, SSC and GF methods. ANN analysis with one input (e.g.  $V$ )  
339 does not perform as good as ( $R^2 = 0.96$  and  $\text{RMSEp} = 0.021 \text{ cm}^3 \text{ cm}^{-3}$ ) the OV method.  
340 However, the ANN performance is the second best after the OV method. The worst  
341 performing methods are the SSC and M with the largest RMSEp values of 0.026 and 0.025  
342  $\text{cm}^3 \text{ cm}^{-3}$ , respectively. Cosh et al. (2005) compared the performance of the M and SSC

343 methods using 180 samples collected from arable and grassland sites with a wide range of  
344 soil texture. They reported a smaller RMSEp value with SSC ( $0.040 \text{ cm}^3 \text{ cm}^{-3}$ ), as compared  
345 to M ( $0.053 \text{ cm}^3 \text{ cm}^{-3}$ ). This RMSEp range is overall larger than that obtained in the current  
346 study, although we accounted for different textures, OM and land use (Table 4).

347 The ANN calibration method based on data fusion generally provides better measurement of  
348  $\theta_v$ , with best results obtained when both V and vis-NIR spectra were used as input data  
349 (Table 3) for training ( $R^2 = 0.98$  and  $\text{RMSEp} = 0.015 \text{ cm}^3 \text{ cm}^{-3}$ ), in comparison with the M,  
350 GF, SSC, OV and ANN-V models. Furthermore, this ANN-data fusion analysis with V and  
351 spectra only performs the best among other ANN data-fusion analyses, where texture  
352 fractions and OM were used as input together with V and spectra (Table 4). In addition to the  
353 fact that the ANN – data fusion model results in the best measurement accuracy of  $\theta_v$ , a  
354 shorter time was needed to conduct ANN calibration-prediction, as compared to the single  
355 input modelling methods. This technique requires only V and soil spectra to be used as input  
356 data, which are anyway measured by ThetaProbe and vis-NIRS, respectively.

357 After the ANN – data fusion model, the OV calibration model with one input variable (e.g. V)  
358 can be ranked as the second best predicting of  $\theta_v$  (Table 4), when validated with the  
359 independent validation set. By using 75% (759 samples) of the total 1013 soil samples, the  
360 following 2<sup>nd</sup> order polynomial equation is established with OV method (Fig. 5):

361

$$362 \quad \theta_v = 0.52V^2 - 0.161V + 0.141 \quad (8)$$

363

364

365 Equation (8) is based on wide variations in soil type, moisture content, OM and land use  
366 (Table 1) of UK soils. Therefore, it is an improved regression equation as compared, for  
367 example with that reported by Kaleita et al. (2005), who attempted to relate  $\theta_v$  with K, using

368 a smaller number of 100 samples only. Their regression models resulted in  $R^2$  values of 0.85  
369 and 0.77 for the laboratory and *in situ* experiments, respectively. The GF regression equation  
370 of Topp et al. (1980) based on soil samples collected from all over the world, provided an  
371 adequate estimation of  $\theta_v$  in the range  $<0.5 \text{ cm}^3 \text{ cm}^{-3}$ , which covers the entire range of  
372 interest in most mineral soils, with a RMSEp of  $0.013 \text{ cm}^3 \text{ cm}^{-3}$ . Jones et al. (2002) reported a  
373 shortcoming of GF method for  $\theta_v$  exceeding  $0.5 \text{ cm}^3 \text{ cm}^{-3}$  in organic or mineral soils with  
374 high OM or C content. The GF regression equation results in a slightly smaller accuracy  
375 (RMSEp =  $0.020 \text{ cm}^3 \text{ cm}^{-3}$ ), as compared to that (RMSEp =  $0.020 \text{ cm}^3 \text{ cm}^{-3}$ ) obtained with  
376 Eqn. (8), as shown in Table 4.

377

### 378 ***3.2. Accuracy of visible and near infrared spectroscopy for gravimetric moisture content*** 379 ***measurement***

380 When the vis-NIR spectra only used as input data, a smaller measurement accuracy of  $\omega$  was  
381 obtained with the PLSR model ( $R^2 = 0.91$  and RMSEp =  $0.027 \text{ g g}^{-1}$ ), as compared to the  
382 ANN model ( $R^2 = 0.95$  and RMSEp =  $0.020 \text{ g g}^{-1}$ ) (Table 4). This is expected results, as  
383 ANN has been proved to over-perform PLSR for the measurement of soil properties with vis-  
384 NIRS (Khalilmoghadam et al., 2009; Mouazen et al., 2010; Viscarra Rossel and Behrens,  
385 2010; Quraishi and Mouazen, 2013b). However, this is a clear contradict to the measurement  
386 of  $\theta_v$ . ANN – data fusion based analysis results in much improved measurement performance  
387 of  $\omega$ , as compared to PLSR technique. Furthermore, ANN – data fusion modelling based on  
388  $V$  and spectra, over-performs ( $R^2 = 0.98$  and RMSEp =  $0.014 \text{ g g}^{-1}$ ) all other ANN – data  
389 fusion analyses based not only on  $V$  and spectra only, but laboratory measured texture  
390 fractions and OM (Table 4). After ANN – data fusion model based on  $V$  and spectra, the best  
391 second performing techniques are those based either on the fusion of  $V$ , spectra and OM or  $V$ ,  
392 spectra and C ( $R^2 = 0.96$  and RMSEp =  $0.018 \text{ g g}^{-1}$ ).



393 High correlation between ANN – data fusion (e.g.  $V$  and soil spectra) measured and oven  
394 drying measured  $\omega$  can be observed in Fig. (6B). This correlation is much improved as  
395 compared to that after PLSR (Fig. 6A), which exhibits non-linear behaviour. Since ANN was  
396 reported to solve problems with non-linear behaviours such as that shown in Fig. (6A)  
397 (Mouazen et al., 2010; Viscarra Rossel and Behrins, 2010), this non-linear behaviour  
398 disappeared in Fig. (6B) after ANN – data fusion modelling. The ANN – data fusion results  
399 in a RPD value of 4.45 for the independent validation set, which can be classified as excellent  
400 measurement performance according to Mouazen et al. (2006b), although the PLSR also  
401 results in an excellent but smaller RPD value of 3.57. Mouazen et al., (2006a) stated that the  
402 performance of vis-NIRS-PLSR to predict  $\omega$  is influenced by the scale of modelling. They  
403 reported a lower validation accuracy for a sample set collected from multiple fields in  
404 Belgium and northern France ( $R^2 = 0.91$  and RPD = 3.22), as compared to that of a single-  
405 field sample set ( $R^2 = 0.97$  and RPD = 5.26). The accuracy of measurement obtained in the  
406 current study with both PLSR and ANN – data fusion for a sample set collected from 32  
407 fields in the UK is higher than that reported by Mouazen et al. (2006a), which is encouraging  
408 result to suggest using the current  $\omega$  models for BD assessment. Likewise for  $\theta_v$   
409 measurement, ANN – data fusion technique provides the best  $\omega$  measurement performance,  
410 and requires the same input of  $V$  and soil spectra only (Table 4).

411

### 412 **3.3. Bulk density assessment**

413 Having  $\omega$  and  $\theta_v$  measured accurately, respectively with the vis-NIRS and ThetaProbe, they  
414 are substituted in Eqn. (1) to derive BD. The accuracy of BD assessment with a single input  
415 variable (e.g.  $V$  or soil spectra) or with multiple input variables (e.g.  $V$ , soil spectra, C, S, SL  
416 and OM) (Table 3) is discussed in the following sections.

417

### 418 **3.3.1 Accuracy of bulk density assessment with a single input variable**

419 Under this BD modelling category,  $\omega$  is measured based on vis-NIR spectra - PLSR, whereas  
420  $\theta_v$  is measured based on  $V$  only and by means of the five calibration techniques of  
421 ThetaProbe discussed above. Generally, the BD assessment in this category is not  
422 encouraging ( $R^2 = 0.23 - 0.53$  and  $RMSEp = 0.160 - 0.190 \text{ g cm}^{-3}$ ). The best assessment is  
423 obtained with ANN - moisture content model ( $R^2 = 0.69$  and  $RMSEp = 0.122 \text{ g cm}^{-3}$ ),  
424 however, this is still with a relatively high  $RMSEp$  (Table 4). Figure 7A illustrates the scatter  
425 plots of estimated BD with ANN – single input variable moisture content models versus oven  
426 drying measured BD. This is still valuable results, as the analysis is capable to predict BD of  
427 soils with a wide range of BD variation between 1.0 and 2.0  $\text{g cm}^{-3}$ . The intercept of the  
428 linear regression equation reveals that the new system over-estimates BD, which might be  
429 attributed to the relatively low accuracy of the vis-NIRS for the measurement of  $\omega$ , as  
430 compared to the ThetaProbe for the measurement of  $\theta_v$ .

431

### 432 **3.3.2 Accuracy of bulk density assessment with multiple input variables (data fusion)**

433 Under this modelling category, both  $\omega$  and  $\theta_v$  are predicted with ANN based on different  
434 combinations of input variables of vis-NIR spectra,  $V$ ,  $S$ ,  $SL$ ,  $C$  and  $OM$  (Table 3). Generally,  
435 as for the measurement performance of  $\omega$  and  $\theta_v$ , the assessment of BD (using Eqn. 1) with  
436 ANN – data fusion techniques ( $R^2 = 0.65 - 0.81$  and  $RMSEp = 0.127 - 0.095 \text{ g cm}^{-3}$ ) over-  
437 performs the corresponding assessments obtained with the single input variable methods ( $R^2$   
438  $= 0.23 - 0.53$  and  $RMSEp = 0.160 - 0.187 \text{ g cm}^{-3}$ ) (Table 4). These results are in agreement  
439 with those reported by Quraishi and Mouazen (2013b). Although high assessment accuracy  
440 of BD is obtained with different  $\omega$  and  $\theta_v$  models of ANN – data fusion with different  
441 combination of input variables, the accuracy increases with the decrease in the number of  
442 input variable used for  $\omega$  and  $\theta_v$  analyses. This trend is clearly illustrated by the increase in

443 RMSEp values with the number of input variables used during ANN analyses (Fig. 8C) of the  
444 independent validation set. However,  $R^2$  values decrease with the increase in the number of  
445 input variable (Fig. 9). This trend can be attributed to a similar trend observed for  $\theta_v$  (Figs.  
446 8A and 9) and  $\omega$  (Figs. 8B and 9). One exception is for the ANN model based on  $V$ , spectra,  
447 C and OM input variables, for which smaller accuracy can be observed, as compared to those  
448 obtained with a larger number of input variables (Figs. 8 & 9). Furthermore, ANN – data  
449 fusion model with  $V$ , Spec and C is less performing, as compared to that with  $V$ , Spectra and  
450 OM (Figs. 8 & 9). Among all models, the ANN - data fusion with  $V$  and soil spectra only  
451 used as input variables for the measurement of  $\omega$  and  $\theta_v$  performs the best for the assessment  
452 of BD using Eqn. (1) ( $R^2 = 0.81$  and  $RMSEp = 0.095 \text{ g cm}^{-3}$ ). This is mainly attributed to a  
453 much larger improvement in  $\omega$  measurement, as compared to  $\theta_v$  (Table 4), when ANN is  
454 used. This model provides useful information about field BD with small RMSEp, to  
455 recommend practical application of the new proposed system of combining vis-NIRS and  
456 FDR for the assessment of BD.

457

#### 458 **4. Conclusions**

459 The visible and near infrared spectroscopy (vis-NIRS) for the measurement of the gravimetric  
460 moisture content ( $\omega$ ) was combined with the ThetaProbe for the measurement of the  
461 volumetric moisture content ( $\theta_v$ ) for *in situ* assessment of soil bulk density (BD). From the  
462 results obtained for 32 fields in the UK with different texture, organic matter, moisture  
463 contents, and land use, the following conclusions were drawn:

- 464 1- Soil BD can be measured with the proposed new approach by substituting the vis-NIR  
465 measured  $\omega$  and the ThetaProbe predicted  $\theta_v$  into an existed BD model with a high accuracy.
- 466 2- The accuracy of BD assessment depends on the measurement accuracy of  $\omega$  and  $\theta_v$ . The  
467 highest accuracy ( $R^2 = 0.81$  and  $RMSEp = 0.095 \text{ g cm}^{-3}$ ) was based on  $\omega$  and  $\theta_v$  values

468 predicted with artificial neural network (ANN) – data fusion models with ThetaProbe output  
469 voltage ( $V$ ) and vis-NIRS spectra used as input variables.

470 2- The performance of the BD model based on ANN – data fusion approach deteriorated with  
471 the number of input variables used to predict  $\omega$  and  $\theta_v$ .

472 A further research is being undertaken to improve the calibration of the ANN models, by  
473 understanding and quantifying the effects of moisture, texture and land use on the  
474 measurement accuracy. Investigation is being undertaken to develop a portable system by  
475 implementing the results achieved in the current work.

476

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480

## 481 **6. References**

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