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

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Abstract

This paper introduces a new approach for the assessment of soil bulk density (BD), which relies on an existed model to predict BD as a function of a visible and near infrared spectroscopy (vis-NIRS) measured gravimetric moisture content (ω) and a frequency domain reflectometry (FDR) measured volumetric moisture content (θv). A total of 1013 soil samples collected from England and Wales, from 32 arable and grassland fields with different soil types were measured with a vis-NIR spectrophotometer (LabSpec®Pro Near Infrared Analyzer, Analytical Spectral Devices, Inc, USA) after *in situ* measurement with a ThetaProbe FDR (Delta-T Device Ltd). Two calibration methods of the vis-NIRS were tested, namely, partial least squares regression (PLSR) and artificial neural network (ANN). ThetaProbe calibration was performed with traditional methods and ANN. ANN analyses were based on a single input or multiple input variables (data fusion). During ANN - data fusion analysis, vis-NIRS spectra and ThetaProbe output voltage (V) were fused in one matrix with or without laboratory measured texture fractions and organic matter content (OM). For the vis-NIRS and ThetaProbe traditional calibration, samples were divided into calibration (75 %) and prediction (25 %) sets, whereas for the ANN analysis these were divided into calibration (65%), test (10%) and independent validation (25%) sets. Results proved that high measurement accuracy can be obtained for ω and θv with PLSR and the best performing traditional calibration method of the ThetaProbe with R^2 values of 0.91 and 0.97, and root mean square error of prediction (RMSEp) of 0.027 g g^{-1} and 0.019 cm^3 cm^{-3}, respectively. However, the ANN – data fusion resulted in improved accuracy (R^2 = 0.98 and RMSEp = 0.014 g g^{-1} and 0.015 cm^3 cm^{-3}, respectively). This data fusion approach led to the best accuracy for BD assessment when vis-NIRS spectra and ThetaProbe V only were used as input data (R^2 = 0.81 and RMSEp = 0.095 g cm^{-3}). It can be concluded that BD can be measured by combining the vis-NIRS and FDR techniques based on ANN-data fusion approach.

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

1. Introduction

Forest, arable and grasslands are important natural resources, which have been subjected to artificial and natural compression stresses through the ages. Heavy agriculture machinery, intensive use of the arable lands and livestock impact on grasslands during the wet soil conditions, are among the major factors causing compression stresses, which lead to soil compaction (Vrindts et al., 2005). Soil compaction is normally associated with damage of the soil structure, deterioration of physical and hydraulic properties and creation of unfavourable conditions for plant root system. Compacted soils demand large amount of fertilisers, in order to substitute the small volume available for plant roots, which might cause contamination hazardous of the ground water by the deep percolation or the run off to the surface water (Soane and van Ouwerkerk, 1995). Highly compacted soils can be considerably of low productivity and require more mechanical power for soil preparations. Among other parameters used to assess soil compaction, bulk density (BD) that is the closer packing of solid particles or the reduction in porosity is a widely used parameter (Grossman, 1981; Bardy, 1984; Singh et al., 1992; Wuest et al., 2009). However, BD might be considered as a sing of soil compaction, as it does not necessarily reflect soil functioning (e.g. air and water movement) (Quraishi and Mouazen, 2013a). Other parameters e.g. saturated hydraulic conductivity and infiltration rate are more closely related to soil compaction (Fleige and Horn, 2000), as compared to BD. However, in comparison with the latter parameters, assessment of BD with a portable system is possible (Quraishi and Mouazen, 2013a) and enables faster, easier and more cost effective data acquisition, which is particularly useful for precision agriculture applications.

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

For years, visible and near infrared spectroscopy (vis-NIRS) has provided a proven and versatile analytical method for soil analyses (Viscarra Rossel & McBratney, 1998; Shepherd & Walsh, 2002; Clark et al, 2005; Mouazen et al, 2010; Stenberg et al., 2010). It is fast measurement technique, non-destructive and cost effective (Mouazen et al., 2005). It was successfully used to measure gravimetric moisture content (ω) under laboratory non-mobile measurement conditions (Dalal and Henry, 1986; Slaughter et al., 2001; Lobell and Anser, 2002; Mouazen et al., 2006a) and on-line mobile conditions (Mouazen et al., 2005). These successful applications were attributed to the strong influence of O-H bond on vis-NIR spectra of soils (Kuang et al., 2012; Stenberg et al., 2010).

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

Multiple sensor and data fusion is being introduced as a new concept in proximal soil sensing (Kuang et al., 2012). Data fusion is an important tool that may improve the performance of a detecting system while various integrated sensors are available (Mahmood et al., 2009). Despite the fact that this is a new concept, several studies were reported for non-mobile (Hummel et al., 2004; Quraishi and Mouazen, 2013b) and mobile (Glancey et al., 1989; Mouazen et al., 2003; Adamchuk et al., 2004; Mouazen et al., 2005; Mouazen and Ramon, 2006; Naderi-Boldaji et al., 2012; Quraishi and Mouazen, 2013c) measurement conditions. Quraishi and Mouazen (2013b) reported a data fusion approach of BD assessment, based on the fusion of data on ω, OM and clay content (C), measured with a vis-NIR spectrophotometer and penetration resistance measured with a penetrometer. However, a large number of variables e.g. ω, OM, C and penetration resistance is needed as input for the artificial neural network (ANN) to predict BD is required. The accumulated error of vis-NIR measurement of ω, OM and C would sum up to a considerable error of BD assessment. Therefore, a simpler approach is needed that is based on a fusion of fewer input variables (e.g. ω and θv), where error in BD assessment is small.

The aim of the paper is to introduce a new approach for BD assessment to be adopted for precision agriculture applications, which is based on a multi-sensor and data fusion approach. It relays on combining the vis-NIRS measurement of ω and ThetaProbe measurement of θv, which are substituted into an existed model to predict BD.

2. Materials and methods

2.1. Experimental sites and soil samples

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

2.2. Laboratory analysis

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

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

2.3. Soil bulk density estimation

The following relationship exists between BD, ω and θv (Wijaya et al., 2004):

$$BD = \theta \mathrm{v} / \omega \tag{1}$$

Where: BD is the soil bulk density in g cm^{-3}, θv is the volumetric moisture content in cm^3 cm^{-3} and ω is the gravimetric moisture content in g g^{-1}.

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

2.4. ThetaProbe and visible and near infrared spectroscopy

A ThetaProbe and a vis-NIR spectrophotometer were used to measure θv and ω, respectively. A detailed description of the measurement is provided in the following subsections.

2.4.1. ThetaProbe description

ThetaProbe (Delta-T Devices Ltd., 1999) is the commercial name of dielectric probe to measure θv. It has been developed jointly by the Macauley Land Use Research Institute, Scotland and Delta-T Devices Ltd, Cambridge. ThetaProbe consists of waterproof housing, which contains electronic circuit attached to it at one end, and four parallel stainless steel rods of 60 mm long and 3 mm in diameter, to be inserted into the soil and at the other end input/output cable (Fig. 2). The electronic circuit generates and emits electromagnetic signal of sinusoidal shape, which is applied to an internal transmission line to the array of four rods. The impedance of this array varies according to the impedance of the soil, which has two components, namely, the apparent dielectric constant (*K*) and the ionic conductivity. A 100 MHz of frequency was chosen in order to minimise the effect of ionic conductivity, so that changes in the transmission line impedance dependent almost solely on the soil's apparent *K*. Water content determines *K* of the soil, as *K* of the water (~81) is much higher than *K* of the soil (3 to 5) and that of the air (1). The traveling electromagnetic wave through the soil mass will cause a voltage standing wave to be set up from the interference of the emitted signal and its reflected component. By measuring this voltage amplitude, *K* of the soil can be obtained and thus θv. More details can be found in Gaskin in Miler (1996) and Miller and Gaskin (1997). Kaleita et al. (2005) studied the effect of soil temperature on laboratory calibration of ThetaProbe, and found insignificantly differences in the accuracy for a temperature range of 10 to 40 °C. Insignificant effect of soil salinity in the range of 250 - 2000 mS m^{-1} was confirmed by the ThetaProbe manufacturer (Delta-T Devices Ltd., 1999).

2.4.2. ThetaProbe calibration and validation

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

2.4.2.1. Manufacturer calibration method (M)

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

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

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

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

$$\theta\text{v} = \frac{\sqrt{k} - 1.6}{8.4} \qquad (3)$$

$$\theta\text{v} = \frac{\sqrt{k} - 1.3}{7.7} \qquad (4)$$

2.4.2.2. Specific soil calibration method (SSC)

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

$$\theta\text{v} = \frac{\sqrt{K} - a_0}{a_1} \qquad (5)$$

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

$$a_1 = \frac{\sqrt{K_1} - \sqrt{K_0}}{\theta \mathrm{vt}} \tag{6}$$

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

2.4.2.3. General formula calibration method (GF)

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

$$\theta \mathrm{v} = -0.053 + 0.0292K - 0.00055K^2 + 0.0000043K^3 \tag{7}$$

The *K* value is derived based on average measured *V*, which is substituted into Eqn. 7. to calculate θv.

2.4.2.4. Output voltage calibration method (OV)

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

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

2.5. Visible and near infrared spectrophotometer calibration and validation

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

2.5.1. Spectra pre-treatment and establishment of calibration model

Spectra pre-treatment aimed to reduce spurious peaks that do not contain physical or chemical information and to correct physical scatter effects. Soil spectra range was first reduced to 500– 2200 nm, to eliminate noise at both edges and to enhance calibration accuracy for ω measurement (Mouazen et al., 2005). After noise cut, spectra were reduced by averaging 10 successive wavelengths. Maximum normalisation was followed, which is typically used to get all data to approximately the same scale, or to get a more even distribution of the variances and the average values. The maximum normalisation is a normalisation that "polarizes" the spectra. The peaks of all spectra with positive values were scaled to + 1, while spectra with negative values were scaled to − 1. Since soil spectra have maximum positive values, the peaks of these spectra were scaled to + 1 (Mouazen et al., 2005). The maximum normalisation led to better results for ω measurement, compared to other pre-treatment options tested. Spectra were then subjected to Savitzky–Golay first derivation transformation (Martens and Naes, 1989). This method enables to compute the first or higher order derivatives, including a smoothing factor, which determines how many adjacent variables will be used to estimate the polynomial approximation used for derivatives. A second order polynomial approximation was selected. A 2:2 smoothing was carried out after the first derivative to decrease noise from the measured spectra. All pre-treatment steps were carried out using Unscrambler 7.8 software (Camo Inc.; Oslo, Norway).

The entire 1013 soil spectra were divided into calibration (75%) and independent validation (25%) sets. Partial least squares regression (PLSR) was implemented using the calibration set to relate the variation in one response variable (e.g. ω) to the variation in multi-spectra wavelengths, using Unscrambler 7.8 software (Camo Inc.; Oslo, Norway). It is a bilinear modelling method where information in the original x data is projected onto a small number of underlying ("latent") variables called PLS components. The y data are actively used in estimating the "latent" variables to ensure that the first components are those that are most relevant for predicting the y variables. Interpretation of the relationship between x data and y data is then simplified as this relationship is concentrated on the smallest possible number of components. More detailed information about the PLSR can be found in Martens and Naes (1989).

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

2.6. Data fusion and modelling

Methods adopted in sections 2.2. and 2.3. for the measurement of θv and ω, respectively, were based solely on output signal of ThetaProbe or vis-NIRS, respectively. In this section, the measurement of θv and ω is based on fusion of output data from both sensing techniques (*V* and spectra) with or without data obtained from laboratory analysis on sand (S in %), silt (SL in %), C in % and OM in %. However, in order to compare with other data fusion models, input data of V or soil spectra were used for the measurement of θv and ω, respectively.

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

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

3. Results and discussion

3.1. Accuracy of ThetaProbe measurement for volumetric moisture content

Table 4 shows the results of the measurement accuracy of θv with the ThetaProbe against the oven drying method using M, SSC, GF, OV and ANN calibration models with one input parameter (e.g. output voltage V). Results suggest that the ThetaProbe is capable to measure θv with high accuracy even with the M calibration method, without the need for additional calibration. However, slight differences can be observed between these methods. With the M method, the measured values of θv overestimate the oven drying measured values. Working with M method, Robinson et al. (1999) and Kaleita et al. (2005) observed similar overestimation for a group of soil samples across a full range of moisture content. Both research groups indicated that the accuracy of the ThetaProbe declined with moisture content, which is a similar trend observed in the current study. The scatter plot of the ThetaProbe-M predicted versus oven drying measured θv illustrates intercept with x axis with a value of 1.12 cm^3 cm^{-3}, indicating overestimation of the M model (Fig. 4). The SSC calibration method performs as equal as that of the M method. However, the GF calibration method provide an improved measurement accuracy (R^2 = 0.96 and RMSEp = 0.020 cm^3 cm^{-3}) (Table 4). The RMSEp obtained with these three methods (e.g. M, SSC and GF) is still larger than 0.01 m^3 m^{-3}, which contradicts the instruction provided by the ThetaProbe's manufacturer. The OV calibration method leads to further improvement (R^2 = 0.97 and RMSEp = 0.019 cm^3 cm^{-3}), as compared to the M, SSC and GF methods. ANN analysis with one input (e.g. V) does not perform as good as (R^2 = 0.96 and RMSEp = 0.021 cm^3 cm^{-3}) the OV method. However, the ANN performance is the second best after the OV method. The worst performing methods are the SSC and M with the largest RMSEp values of 0.026 and 0.025 $cm^{-3}cm^{-3}$, respectively. Cosh et al. (2005) compared the performance of the M and SSC methods using 180 samples collected from arable and grassland sites with a wide range of soil texture. They reported a smaller RMSEp value with SSC (0.040 cm^3 cm^{-3}), as compared to M (0.053 cm^3 cm^{-3}). This RMSEp range is overall larger than that obtained in the current study, although we accounted for different textures, OM and land use (Table 4).

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

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

$$\theta \mathrm{v} = 0.52V^2 - 0.161V + 0.141 \tag{8}$$

Equation (8) is based on wide variations in soil type, moisture content, OM and land use (Table 1) of UK soils. Therefore, it is an improved regression equation as compared, for example with that reported by Kaleita et al. (2005), who attempted to relate θv with *K*, using a smaller number of 100 samples only. Their regression models resulted in R^2 values of 0.85 and 0.77 for the laboratory and *in situ* experiments, respectively. The GF regression equation of Topp et al. (1980) based on soil samples collected from all over the world, provided an adequate estimation of θv in the range <0.5 cm^3 cm^{-3}, which covers the entire range of interest in most mineral soils, with a RMSEp of 0.013 cm^3 cm^{-3}. Jones et al. (2002) reported a shortcoming of GF method for θv exceeding 0.5 cm^3 cm^{-3} in organic or mineral soils with high OM or C content. The GF regression equation results in a slightly smaller accuracy (RMSEp = 0.020 cm^3 cm^{-3}), as compared to that (RMSEp = 0.020 cm^3 cm^{-3}) obtained with Eqn. (8), as shown in Table 4.

3.2. Accuracy of visible and near infrared spectroscopy for gravimetric moisture content measurement

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

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

3.3. Bulk density **assessment**

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

3.3.1 Accuracy of bulk density assessment with a single input variable

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

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

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

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

4. Conclusions

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

1- Soil BD can be measured with the proposed new approach by substituting the vis-NIR measured ω and the ThetaProbe predicted θv into an existed BD model with a high accuracy.

2- The accuracy of BD assessment depends on the measurement accuracy of ω and θv. The highest accuracy (R^2 = 0.81 and RMSEp = 0.095 g cm^{-3}) was based on ω and θv values predicted with artificial neural network (ANN) – data fusion models with ThetaProbe output voltage (*V*) and vis-NIRS spectra used as input variables.

2- The performance of the BD model based on ANN – data fusion approach deteriorated with the number of input variables used to predict ω and θv.

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

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

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