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**Development of Micro-Tractor-based Measurement  
Device of Soil Organic Matter using on-the-go Visual-  
Near Infrared Spectroscopy in Paddy Fields of South  
China**

**Lianqing Z, Zhou S, Songchao C, Yafei Y**

Institute of Remote Sensing and Information System, College of Environmental &  
Resources Science, Zhejiang University, Hangzhou 310058, China

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**Abstract.** Soil organic matter (SOM) is an essential soil property for assessing the fertility of paddy soils in South China. In this study, a set of micro-tractor-based on-the-go device was developed and integrated to measure in-situ soil visible and near infrared (VIS-NIR) spectroscopy and estimate SOM content. This micro-tractor-based on-the-go device is composed of a micro-tractor with toothed-caterpillar band, a USB2000+ VIS-NIR spectroscopy detector, a self-customized steel plow and a self-customized compact spectroscopy probe with a sapphire windows. Two study area are selected, one is located in Hunan, the other in Jiangxi provinces, P. R. China. In each study area, vis-NIR spectra of 50 sites were collected by on-the-go spectroscopy detector and the corresponding topsoil were collected using a cubic soil sampler (10 cm×10 cm×20 cm). Then soil samples were air dried, ground and sieved to a size fraction of less than 2 mm. SOM was measured using the H<sub>2</sub>SO<sub>4</sub>-K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> oxidation method at 180 °C for 5 minutes and VIS-NIR spectra were measured again in the laboratory condition using an USB2000+ linked to a laptop by an USB cable. Based on laboratory spectra, direct standardization (DS) method was applied to remove environmental factors from field spectra. The resulting data were divided into calibration (34 samples) and validation (16 samples) sets in two fields, respectively. A partial least square regression (PLSR) was used to predict SOM using on-the-go spectra, laboratory spectra and DS-transferred spectra. SOM spatial distribution maps developed using the on-the-go measured VIS-NIR spectra and the laboratory measured validation dataset were compared. Being interfered by environmental factors, especially water in the soil, the prediction accuracy of SOM using on-the-go spectra (RPD between 0.9995 and 1.3561) were less than these using laboratory spectra (RPD between 1.7747 and 1.8981).

*Predictions of SOM with the DS-transferred spectra (RPD between 1.6261 and 1.6671) were more accurate than these with on-the-go spectra. Both of two maps showed partial similarity at most areas over two fields. Research results indicated a great potential to estimate SOM in the field using our on-the-go vis-NIR spectroscopy platform combing DS method.*

**Keywords.**

*Soil Organic Matter, on-the-go, Visual-Near Infrared Spectroscopy, Paddy Fields*

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## Introduction

Rice is the typical product of paddy soils and the main food for people in China. So paddy soils are very important in China and widely distributed mainly in the south of China, especially in the Yangtze River Delta area of China. As one of the major rice producers, China has a large area of paddy fields of more than 25 million hectares, accounting for 29% of the cultivated lands of China and 23% of the world (Ji et al., 2014). Soil organic matter (SOM) is an essential factor in rice growth, as it affects soil moisture infiltration and retention, soil tilth, rooting depth, soil-applied herbicide activity, nitrogen release, and other aspects of nutrient cycling in paddy soils in South China. It plays a great deal of part in soil fertility, rural ecological-environment protection and sustainable development of rice production. Therefore, accurate characterization of the spatial variability of SOM in paddy soils is essential for fertilizer recommendation, digital soil mapping, and information making for precision agriculture.

Over the past decades, various sensors have been used to determine the content of SOM. Among these sensors, proximal soil sensing with visible and near-infrared (VIS-NIR) spectroscopy provides a potential tool to measure SOM of paddy soils because it enables rapid, less labor-intensive and cost-effective measurement compared to conventional chemistry experiment (Li et al. 2015). SOM was successfully measured with non-mobile NIR spectroscopy. However, these studies were carried out in a non-mobile (laboratory) environment, where soil samples were collected from agricultural fields and treated using conventional methods, and the advantage of obtaining continuous information about SOM cannot be fulfilled. In recent years with more and more built-in computer, optic, spectroscopy and other high technologies were introduced to precision agriculture, some on-the-go sensors were developed for measure SOM. Shonk et al. (1991) developed a prototype real-time soil organic matter sensor. This sensor consists of compact transmitter and receiver modules which utilize light reflectance to measure percentage organic matter. Laboratory tests were conducted to determine optimal light wavelengths for use with typical landscapes in the midwestern United States. Preliminary field tests have proven successful for soils ranging from below 1% to over 6% organic matter. They found that soil moisture content significantly affected the sensor output. Christy (2008) developed a soil reflectance mapping unit using a shank-based VIS and NIR spectrophotometers for in situ measurement of reflectance spectra. The best one-field-out validation results were obtained for organic matter (OM), which was predicted with a root-mean-square error (RMSE) of 0.52% and a coefficient of determination ( $R^2$ ) of 0.67. Giyoung Kweon (2013) develop an inexpensive on-the-go optical sensor for soil organic matter (OM) sensing. This optical sensor with dual wavelength was evaluated in field tests with RPD of 2 or greater for OM estimation and showed similar results for OM mapping pattern with  $R^2$  as 0.86 compared to a NIR spectrophotometer shank unit.

It is known that under field conditions, some environmental factors, including ambient light, soil moisture content, texture, color, temperature, harsh field conditions, dust, stoniness and surface roughness, can produce a possible source of error, so the development of accurate and robust calibration models based on Vis-NIR spectroscopy is crucial for on-the-go measurement conditions (Waiser et al., 2007). Therefore, numerous researchers work using soil Vis-NIR spectroscopy are limited to within-field scales (Wijaya et al, 2001; Mouazen et al., 2005; Huang et al., 2007). As reported by Stenberg (2010), the calibration scale affects the accuracy of the models developed, and that field-scale modelling provides the greatest accuracy. But Kuang and Mouazen (2011) compared the performance of calibration models for total carbon (TC), total nitrogen (TN) and organic carbon (OC) developed for individual farms with that of general models valid for three farms in the Czech Republic, Germany and Denmark. Except for the Czech Republic farm, individual farm models provided successful calibration for TC, TN and OC, with  $R^2$  of 0.85–0.93 and 0.74–0.96 and RPD of 2.61–3.96 and 2.00–4.95 for the cross-validation and independent validation respectively. General calibration models gave improved prediction accuracies compared with models of farms in the Czech Republic and Germany. To our knowledge there is no published report on the calibration models for

the measurement of SOM using micro-tractor-based on-the-go soil Vis-NIR spectroscopy in China.

The objectives of this research were to: ① investigate the capability of the self-customized on-the-go Vis-NIR spectroscopy detector based on micro tractor measuring SOM content, ② probe the performances of calibration models in two paddy fields in two province in China, ③ compare SOM spatial distribution maps developed using the on-the-go measured VIS-NIR spectra and the laboratory measured validation dataset were compared.

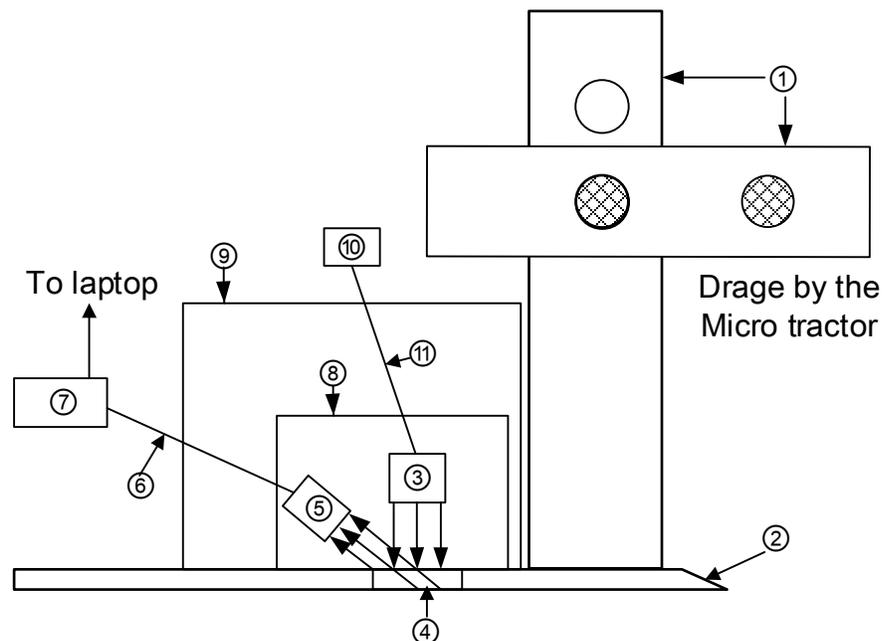
## Materials and methods

### Research fields

Two paddy fields were selected as research fields, one is located in Hunan, the other in Jiangxi provinces, P. R. China. This research work was conducted on 5 Oct. 2015 in Hunan field and 22 Oct. 2015 in Jiangxi field after rice was harvested. At the time of soil spectral data acquisition, in two fields, there was a few amount of rice straw residue still present on the soil surface covering about 10% of the soil surface, and all root of rice straw were buried under the soil surface.

### Micro-tractor-based on-the-go VIS-NIR spectroscopy measurement device

This micro-tractor-based on-the-go device is composed of a USB2000+ fibre type VIS-NIR spectrophotometer (Ocean Optics, Inc., Dunedin, Florida, USA, wavelength ranges from 380nm to 1050nm), a self-customized compact spectroscopy probe with a sapphire windows, a stainless steel plow and a gasoline-powered micro tractor with toothed-caterpillar band (Chinese domestic product) (Fig. 1). The probe is hold within an anti-water stainless-steel holder with a built-in halogen lamp which provide full energy spectroscopy. The probe-hold box is fixed on the horizontal coulter of the micro plow which is fixed on and dragged by the micro-tractor. An optical fiber was used to transfer the reflectance and diffuse reflection spectrum, which passed through the probe sapphire window from soil under the bottom of horizontal coulter, to USB2000+. The USB2000+ was connected to a laptop through a USB cable. A Java-programmed procedure is monitoring the USB2000+ by running on the laptop which was used for data logging and communication. This device, laptop and DGPS were powered by a lithium battery fixed on the micro-tractor.



a



b

**Fig. 1 Micro-tractor-based on-the-go VIS-NIR spectroscopy measurement device. a: is the on-the-go soil spectra detector; b: the device dragged by a gasoline-powered micro tractor with toothed-caterpillar band. ① micro stainless plow; ②subsoiler; ③ halogen lamp;④sapphire window; ⑤ collection optic; ⑥fibre; ⑦USB2000+; ⑧compact probe; ⑨stainless holding box; ⑩lithium battery; ⑪power line**

### **On-the-go soil spectral data acquisition**

There was a stainless steel plow captained by the on-the-go device used in this study. The stainless steel plow consists of a subsoiler that penetrates the paddy soil to the required depth and make a furrow. The furrow bottom is smoothed due to the downwards forces acting on the subsoiler. The probe-hold box is attached to the backside of the subsoiler (Fig. 1) to acquire soil spectra from the smooth bottom of the furrow. Position, latitude and longitude, were determined with a Trimble GeoXT differential global positioning system (DGPS). Each spectrum was an average of ten successive spectra collected along about 1-1.25 m distance, depending on tractor speed.

The field on-the-go measurement was carried out in two fields, one in Hunan province, and the other in Jiangxi province, China. Fields experiments were carried out after harvesting rice. The probe-hold box attached to the backside of the subsoiler was pulled by the micro tractor throughout 4 parallel lines of 4 m apart, parallel with the direction of the tramlines. It was driven at a travel speed of 0.2 m s<sup>-1</sup>, setting the subsoiler tip at a 0.1m depth. After measurement of each line, soil samples were collected from the furrow bottom. These samples were not used for the development of calibration models but as validation set. They were used to produce maps of laboratory reference measurement to be compared with the corresponding maps developed using the on-the-go measured spectra and the laboratory calibration models developed by using on-the-go measured spectra.

### **Laboratory measurements**

After on-the-go measurements, the samples were packed into plastic bags, labeled and transported to laboratory. The soil samples were air-dried, ground and sieved to less than 2 mm. The VIS-NIR spectra of these 100 samples (50 samples for each field) were then measured again under laboratory condition.

An USB2000+ VIS-NIR spectroscopy detector (Ocean Optics, Inc., USA, wavelength ranges from 380nm to 1050nm) was also used for laboratory based measurement. To keep the measurement consistent, the compact probe was also used in the laboratory-based measurement. A Spectralon panel with 99% reflectance was used to calibrate the spectrometer before each measurement.

The chemical analyses of soil properties were also conducted using these samples by the H<sub>2</sub>SO<sub>4</sub>-

K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> oxidation method at 180°C for 5 minutes(Soil Science Society of China, 2000).

### Establishment of calibration models

After pretreated using the Savitzky-Golay algorithm with a window size of 11(Savitzky and Golay, 1964), the results of laboratory chemical analyses were used to develop the calibration models for SOM listed in Table 1. Laboratory measured spectra and on-the-go measured spectra were both divided into either calibration (70%) or independent validation (30%) sets by the Kennard-Stone algorithm (Kennard & Stone, 1969). All on-the-go measured spectra were then subjected to the direct standardization (DS) approach for removing the soil moisture effects. In the next, these spectra were called DS-spectra, these original on-the-go measured spectra were called Raw-spectra. The DS algorithm would be described next. The calibration spectra were subjected to a partial least squares regression (PLSR) with leave-one-out cross-validation using the PLS\_Toolbox8.0.2 (Eigenvector Research Inc., Wenatchee, WA, USA) in Matlab R2009 (MathWorks, Inc., Natick, MA). The number of latent variables for a model was determined by examining a plot of leave-one-out cross-validation residual variance against the number of latent variables obtained from PLSR. The latent variable of the first minimum value of residual variance was selected. Outliers were detected by using the residual sample variance plot after the PLSR. Samples located individually far from the zero line of residual variance were considered to be outliers and were excluded from the analysis. In the next, calibration models developed by laboratory measured spectra calibration were called Lab-calibration models, by DS-spectra were DS-calibration models, by Raw-spectra were Raw-calibration models.

Calibration models were developed for each field separately using samples from each field.

**Table 1. Sample statistics of laboratory results of 50 samples collected from two fields in Hunan and Jiangxi provinces, respectively**

Site	Calibration set				Validation set			
	Min	Max	Mean	Std	Min	Max	Mean	Std
Hunan	12.30	49.70	29.96	10.68	19.50	48.00	29.71	9.45
Jiangxi	10.00	41.00	28.00	9.00	10.00	38.30	30.33	8.24

### The direct standardization (DS) algorithm

The direct standardization (DS) algorithm was first derived by Wang et al. (1991) to correct the difference in spectral response between instruments and the instrument drift. Ji et al. (2015) proposed the use of DS to correct for the effects of soil water and other environmental factors on soil spectra recorded in the field.

In the DS algorithm, a subset of corresponding field (X<sub>F</sub>) and laboratory (X<sub>L</sub>) spectra was first selected from the whole local dataset-the transfer set-to derive the DS transfer matrix, which characterizes the differences between the field and laboratory spectra, written as:

$$X_L = X_F B + E \quad (1)$$

where B is the transfer matrix which accounts for the variation in both X<sub>L</sub> and X<sub>F</sub>, and E is the residual matrix. Once the DS parameters B and E are calculated, the field spectra from the whole local dataset can be transferred by means of the following equation:

$$X'_{Fall} = X_{Fall} + E \quad (2)$$

where X'<sub>Fall</sub> is the field spectra of the whole local dataset and X<sub>Fal</sub> is the transferred field spectra after DS. More details see Ji et al. (2015).

### Partial Least-Squares Regression

Partial least squares regression (PLSR) is one of the most popular multivariate techniques for spectral calibration and prediction(Wold et al, 1983). It is closely related to principal component

regression (PCR) yet with a slight difference. Both of them compress the data before prediction while PLSR avoids the dilemma encountered by PCR of choosing components for the regression. PLSR method reduces the number of variables in the predictor set by selecting successive orthogonal factors from the variance-covariance matrix in a way that maximizes the covariance between the predictors and response variable or variables (there may be more than one variable being predicted). There is a risk of over-fitting or under-fitting, and to avoid this, so the leave-one-out cross-validation method is used to find the optimal number of calibration factors that minimize the prediction error variance. For details, please see Ji et al. (2014)

### Assessment of statistics

Coefficients of determination ( $R^2$ ), root mean square error (RMSE) and the ratio of prediction derivation (RPD) were used to compare the prediction accuracies.

$$R^2 = \frac{\left[ \sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})(y_i - \bar{y}) \right]^2}{\sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})^2 \sum_{i=1}^n (y_i - \bar{y})^2} \quad (3)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2} \quad (4)$$

$$RPD = SD / RMSE \quad (5)$$

Where  $\hat{y}_i$  is the predicted value and  $y_i$  is the observed value,  $\bar{y}$  is the mean of observed value,  $\bar{\hat{y}}$  is the mean of predicted value; SD is standard deviation of observed values, n is the number samples.

Generally, a model that performs well would have large values of  $R^2$  and RPD and a small RMSE, though they are not necessarily monotonically related.

PLS\_Toolbox8.0.2 (Eigenvector Research Inc., Wenatchee, WA, USA) was utilized to preform PLS model in Matlab R2009 (MathWorks, Inc., Natick, MA). SO did Savitzky-Golay algorithm, DS analysis and Kennard-stone algorithm.

## Results

All steps performed in this study, from the collection of soil samples to the development of different maps are illustrated in the flow diagram shown in Fig. 5. This diagram made it clear that the VIS–NIR calibration models were developed using soil spectra measured under non-mobile laboratory environment. The applicability of these laboratory calibration models for on-the-go predictions of soil properties was validated on spectra measured on-the-go with the VIS–NIR sensor.

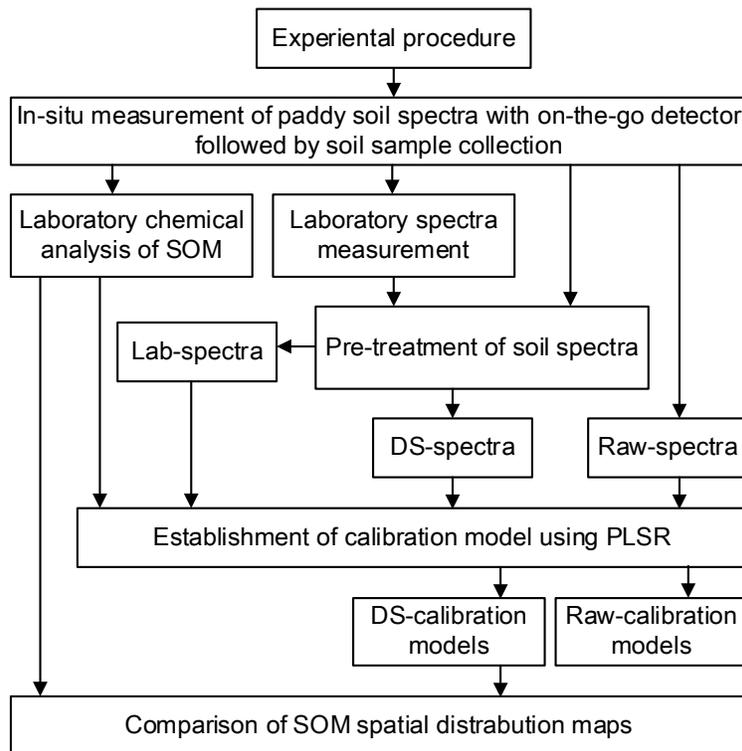


Fig.2 A working flow diagram for different step during this study

### Calibration models for SOM

Calibration models for SOM for two fields were established by PLSR using full cross-validation technique in this study. The adequacy of each SOM calibration model was evaluated  $R^2$  for predicted vs. measured values in cross-validation and prediction, and the RPD. As Mouazen mentioned (2007) that an  $R^2$  value between 0.50 and 0.65 indicates that more than 50% of the variance in Y is accounted for by variable X, an  $R^2$  between 0.66 and 0.81 indicates approximate quantitative predictions, whereas, an  $R^2$  between 0.82 and 0.90 reveals good prediction. If an  $R^2$  is above 0.91 calibration models are considered to be excellent. The RPD indicates that the prediction accuracy has been increased compared to using the mean composition for all samples. RPD is desired to be larger than 2 for a good calibration. A RPD less than 1.5 indicates incorrect predictions and cannot be used for further prediction.

Two calibration models for two files are detailed in Table 2.

Table 2. Results of PLSR for two fields

Site	Raw-calibration models				DS-calibration models				Lab-calibration models			
	LV	$R^2$	RMSE	RPD	LV	$R^2$	RMSE	RPD	LV	$R^2$	RMSE	RPD
Hunan	7	0.4447	9.0511	0.9995	7	0.6321	6.2132	1.6261	9	0.7561	5.0977	1.7747
Jiangxi	10	0.5124	5.9075	1.3561	13	0.6440	4.8053	1.6671	8	0.7314	4.2205	1.8981

\* LV is the number of latent variables in PLSR

According mentioned above, it is clearly showed in Table 2 that both two Raw-calibration models for two fields were lower than 1.5 which indicated incorrect predictions and could not be used for further prediction. DS-calibration models could make approximate quantitative predictions for SOM (RPD was 1.6261 for Hunan field, 1.6671 for Jiangxi field). So did Lab-calibration models (RPD was 1.7741 for Hunan field, 1.8981 for Jiangxi field), and there was little model performance superiority between DS-calibration models and Lab-calibration models.

### Comparison of SOM spatial distribution maps

These two PLSR (7-factor for Hunan field and 13-factor for Jiangxi field) were used to predict SOM of

the 16 field spectra. As might be expected, both PLSR predictions from Hunan and Jiangxi fields made approximate quantitative predictions ( $R^2 = 0.7797$  for Hunan and  $0.6455$  for Jiangxi (as illustrated in Fig. 3).

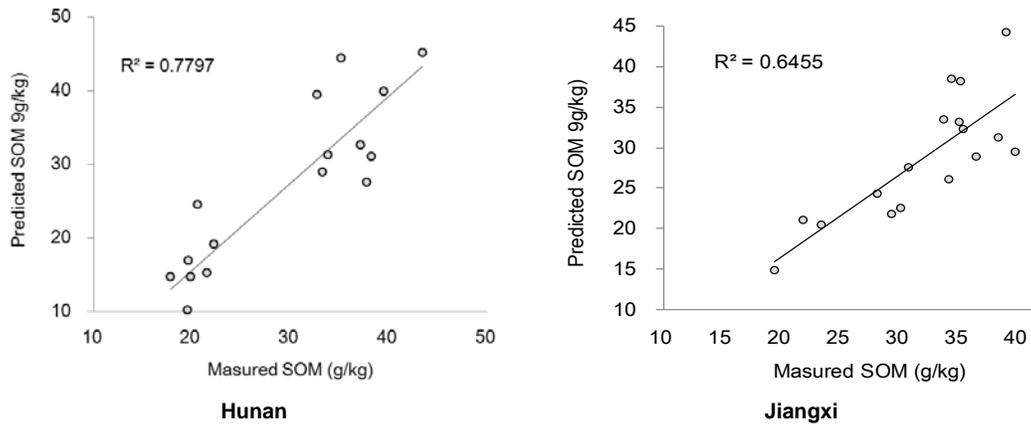


Fig.3 Validation models for two fields

The ESRI ArcMAP 10.1 software was used to draw the SOM spatial distribution map using SOM prediction of spectra measured by the on-the-go detector and the laboratory measured validation dataset. All these maps were developed based on data of a 1 m \* 1 m grid in order to make the resolution of all maps consistent (Fig. 4). The grid was interpolated using the inverse distance weighing (IDW) method.

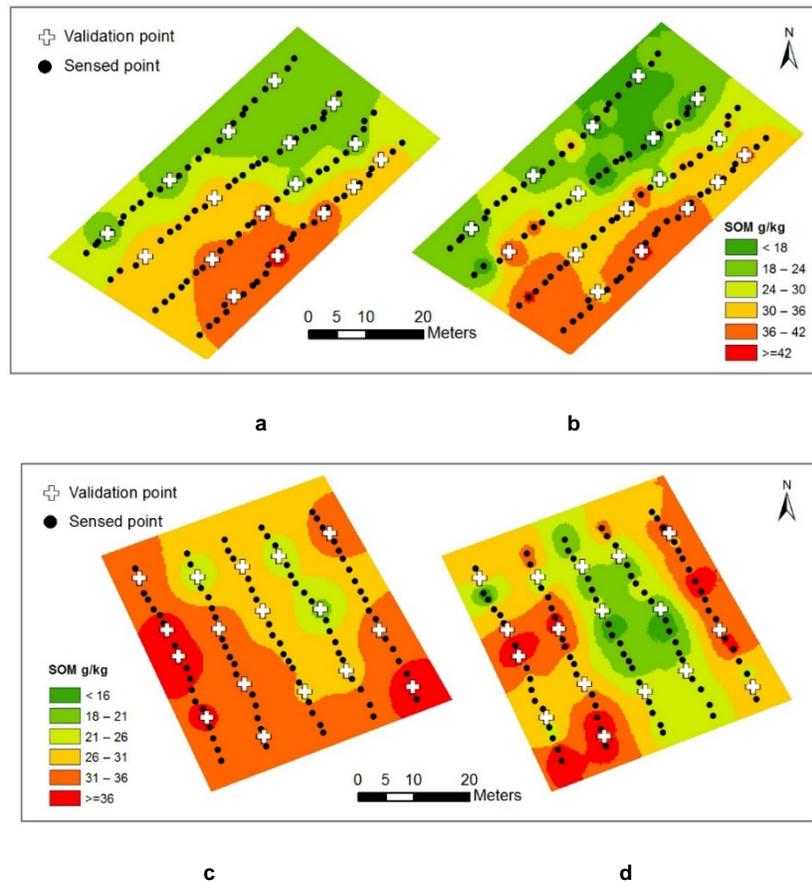


Fig.4 Comparison of reference and (a (Hunan) and c (Jiangxi)) and on-the-go ( b (Hunan) and d (Jiangxi)) measure SOM spatial distribution map

SOM spatial distribution maps developed using the on-the-go measured VIS-NIR spectra were

compared to SOM spatial distribution maps developed using the laboratory measured validation dataset. The PLS calibration models for two fields were utilized to calculate SOM predictions using on-the-go measured soil spectra. The evaluation of the accuracy of on-the-go measured SOM was done by visual comparison between spatial variation of reference and on-the-go measurements. The spatial distribution of SOM measured by the on-the-go device and by the reference methods showed partial similarity at most areas over two fields. The SOM spatial distribution could be adequately detected by using the on-the-go device and the general calibration models. Thus, the on-the-go detecting device could be used to provide relatively consecutive soil spectra to map SOM spatial variation.

## Discussion

Although the calibration models developed for SOM provided approximate quantitative predictions, SOM spatial distribution maps developed using the on-the-go measured VIS-NIR spectra and the laboratory measured validation dataset showed partial similarity at most areas over two fields.

However, the scope of this study was to report a primary investigation of using a self-customized on-the-go VIS-NIR soil spectra detector to measure SOM in two paddy fields of south CHINA. Further research aiming at improving the accuracy and universality of models and the quality of the developed maps is still needed to probe, which would tackle the following points:

1. Use a wider measurement range spectrophotometer: An instrument with a wider wavelength range more than 1050 (the spectrum upper limit of USB2000+ used on this study) even to 2500 is recommended to improve the accuracy of the calibration models, since there may be important SOM absorption features available beyond 1050nm. However, a VIS-NIR spectrophotometer with a wider wavelength range more than 1050 even to 2500 may have a bigger size than USB2000+, and its capital cost may be considerably larger than USB2000+.
2. Improving the calibration models. In this study both two calibration models developed for SOM could provide only approximate quantitative predictions. There were only 34 samples in calibration dataset, which may account for the poor performance of calibration models. In the future research work, it is recommended during calibration to consider more paddy soil samples that comprise more variability in SOM content and more fields.

## Conclusion

A set of micro-tractor-based on-the-go device composed of a USB2000+ spectrometer was used to measure in-situ soil VIS-NIR spectroscopy and estimate SOM content in two fields. Calibration models for two fields were established by PLSR using on-the-go measure soil spectroscopy and laboratory measure references. These calibration models were used to provide quantitative prediction of SOM using soil spectra measured by the on-the-go detector. Both of two models provided approximate quantitative SOM predictions. SOM spatial distribution maps developed using the on-the-go measured VIS-NIR spectra and the laboratory measured validation dataset were compared. Two maps showed partial similarity at most areas over two fields. Thus, the on-the-go detecting device could be used to provide relatively consecutive soil spectra to map SOM spatial variation.

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