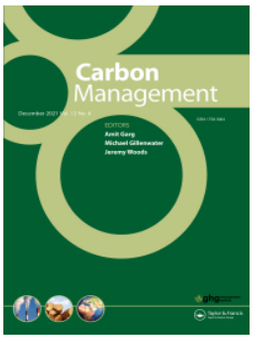

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Assessing the robustness of VIS-NIR spectroscopy-based soil organic carbon prediction against four wet chemistry methods

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ABSTRACT

A visible and near-infrared (VIS-NIR) spectroscopy-based machine learning model can rapidly predict soil organic carbon (SOC) while minimizing environmental impacts once established. Nevertheless, model reliability has mostly been evaluated statistically, with limited explanation from a soil science perspective or validation against various wet lab methods, which differ in reliable. Therefore, this study assessed the robustness of a VIS-NIR-based Cubist model trained with Walkley-Black (WB) SOC data (n = 400) from diverse land uses and soil types in Taiwan. Additionally, SOC contents by total organic carbon (TOC) analyzer, elemental analyzer (EA), and loss-on-ignition (LOI) methods from an independent sample set (n = 46) tested the model's applicability. The model achieved R2=0.72 and RMSE=1.09%, whilst highly aligned with WB measurements (LCCC=0.82). Major model predictors indicated SOC with varying stabilities, where degradation was linked to weathering and stabilization to iron oxides. Predicted SOC contents also aligned with TOC (LCCC = 0.81) and EA (LCCC = 0.76), but less with LOI (LCCC = 0.48) due to overestimation from structural water loss. While VIS-NIR model reflected the precision of training data, consistency with other methods supported its utility as a complementary tool for SOC estimation. This study highlighted VIS-NIR spectroscopy's potential in evaluating stabilized carbon pool for carbon monitoring.

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Data mining; green technology; natural carbon sink; proximal sensing

Introduction

Soil organic carbon (SOC) is a crucial soil component of soil health and a sustainable ecosystem, as it sustains soil productivity, supports the microbiome, and controls soil degradation by improving soil structure and nutrient cycling [1]. Thus, SOC abundance has long been regarded as the key indicator for evaluating soil quality. Moreover, soil is the largest carbon (C) sink within the terrestrial ecosystem, with a C stock of approximately 4.0×10^{12} t, which is five to seven times greater than that in the atmosphere and plants [2]. Therefore, increasing SOC levels has been recognized as one of the crucial natural-based solutions for achieving net-zero emission in the last decade [3]. Accordingly, the measurement of SOC has become the key for taking climate actions. For instance, policy-making for net-zero emissions target by public sectors, developing advance carbon fixation technologies by academic communities, or join the carbon trading market after adopting sustainable agricultural practices by landowners [4]. A practical and sensitive technique that can identify the change in SOC contents, in order to reflect the variation of soil carbon sink becomes the prior concern for these interesting parties [3].

The commonly applied schemes for the SOC measurement worldwide are wet chemical approaches, e.g. Walkley-Black method, total organic carbon analyzer (TOC) method, elemental analyzer (EA) method, and loss-on-ignition (LOI) method. These methods generate discrepant SOC values due to their distinct targeted C-containing components in soils, as they rely on different analysis mechanisms. To address the inconsistency, harmonization techniques such as empirical conversion equations, calibration against a reference method, or regional correction factors can be applied to facility SOC data comparability. However, even standard analysis protocol and data quality assurance processes have been conducted, these wet chemistry methods share some practical limitations, such as being time-consuming, costly, and requiring hazard chemicals. These drawbacks pose the encumbrances for high-frequency SOC

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monitoring, which is crucial for tracking SOC variation over time [5].

Visible (VIS)-near infrared (NIR) spectroscopy, covering wavelength ranges of 350–700 nm and 700–2500 nm, respectively, can detect overtones and combinations arising from the molecular vibrations of major functional groups of soil organic matters (SOM), i.e. O-H, C-H, C-O, and N-H, with a minimal sample pretreatment required [6,7]. Moreover, with the application of machine learning algorithms, the key wavenumbers could be extracted from high-dimensional spectral data, shortening the time consumption in interpreting entire spectrum. While compared to traditional statistical methods, machine learning approaches are particularly robust for handling nonlinear relationships between spectral features and SOC contents. The advantages of which assists the development of a simplified reflectance-SOC calibration model based on SOC measurements from conventional wet lab approaches, thereby offer an intuitive scheme with lower environmental impact for rapid SOC screening [8,9]. Consequently, to meet the global trend for developing a handy choice for the efficient SOC measurement in the last decade, considerable VIS-NIR spectrum-based SOC prediction models have been addressed worldwide according to that from different wet chemistry methods [3,4]. For instance, Zhang et al. (2021) reported a model for the Walkley-Black method analyzed SOC using partial least squares regression (PLSR) with a coefficient of determination (R^2) of 0.85 [9–11], based on 255 soils in northwest China; Lucà et al. (2017) built a model for the TOC method measured SOC *via* PLSR with a root mean square error (RMSE) of 0.71, according to 216 soil samples from south Italy [12]; Zhao et al. (2022) constructed a model for the LOI method determined SOC by Cubist regression algorithm with a Lin's concordance correlation coefficient (LCCC) of 0.90, relied on 634 soils from northeast Australia [13]; Seidel et al. (2019) disclosed a model for the EA method evaluated SOC contents using PLSR with a residual prediction deviation (RPD) larger than 4.3, depending on 142 soils from eastern Germany [6].

The quantification of SOC by integrating VIS-NIR spectroscopy and machine-learning algorithms relies on spectra characteristics influenced by the covariation of soil properties, as well as the reference SOC contents which may vary with the employed wet chemical methodology. These factors further contribute to the selection of different predictive wavelengths [5,8]. However, model reliability has mostly been assessed from a chemometrics perspective using statistical measures, with limited evaluation using a soil science opinion. Additionally, the concordance between predicted SOC values and those obtained from various wet chemical methods—each capable of yielding reliable yet slightly different measurements—has barely been elucidated. Given that the methodological discrepancies of the reference methods could lead to uncertainties in SOC predictions, such a validation is necessary. Therefore, to bridge this gap, soils from different land use scenarios (e.g. paddy fields, uplands, and forests) covering diverse soil properties were collected across Taiwan, and the SOC contents were analyzed with four conventional wet lab approaches, i.e. Walkley-Black method, TOC analyzer method, EA method, and LOI method, for building and assessing a VIS-NIR based SOC calibration model. Thus, the aims of this study were to (1) develop and validate a VIS-NIR-based model for predicting SOC content using Walkley-Black method as a reference, (2) interpret the cause-and-effect relationship between key VIS-NIR wavelengths selected for model construction and soil properties related to SOC stability, and (3) evaluate the model's robustness and limitations by comparing the prediction against those measured by conventional wet chemistry methods with diverse analytical precision.

Material and methods

Sample collection

In order to obtain a wide variation of SOC content and their corresponding spectrum characteristics for constructing a prediction model applicable across various contexts. 400 agricultural and forest soil samples in Taiwan were collected as the model developing set, to cover the diverse parent materials and soil types including Entisols, Inceptisols, Vertisols, Spodosols, Alfisols, and Ultisols in the U.S. soil classification system (Table 1; Fig. S1). The soil samples were collected based on their genetic horizons, i.e. A horizons which were the surface soil with the enrichment of SOM, B horizons which were the subsurface soils with clay and iron (Fe) oxide accumulations, and C horizons which were the lower subsurface soils that close to parent materials and without the illuviation of soil colloids. On the other hand, to further test the model practicality, 46 andesite derived agricultural ($n = 26$) and forest ($n = 20$) soils independent from

Table 1. **The number and frequency of soil samples from different land uses, parent materials, soil types, and horizons in the model developing set ($n = 400$).**

	n	Frequency (%)
Land use		
Agricultural soils	214	54
Forest soils	186	47
Parent material		
Granite	15	3.8
Shale	248	62
Andesite	62	16
Mafic	50	13
Ultramafic	25	6.3
Soil type		
Entisols	15	3.8
Inceptisols	249	62
Vertisols	12	3.0
Spodosols	44	11
Alfisols	37	9.3
Ultisols	43	11
Horizon		
A horizon	244	61
B horizon	124	31
C horizon	32	8.0

those adopted in the modeling, were randomly selected and introduced as the blinded experiment samples/testing set, for simulating the model application scenario when facing unknown samples. The testing set contained 87% of Inceptisols and 13% of Ultisols while 16, 28, and 2 of which were from A, B, and C horizons, respectively.

Soil characterization

All soil samples ($n = 446$) were further air-dried, fine ground, and passed through a 10-mesh sieve (< 2 mm) for the laboratory and spectral analyses. Soil samples from the model developing set ($n = 400$) were determined for their particle size distribution using the pipette method [14] and soil pH *via* a glass electrode with a mixture of soil and deionize water (1:1, weight/volume) [15]. The SOC content for the model developing set was measured following the Walkley-Black method [16]. Besides this wet oxidation approach, the SOC content of the model performance testing set was also quantified using the TOC analyzer (multi N/C 2100S, Analytik Jena, Jena, Germany) and EA (UNICUBE, Elementar, Hanau, Germany) after applying the dry combustion method according to ISO 10694:1995 [17], as well as *via* LOI method [18] (Figure 1; Fig. S2).

VIS-NIR spectrum acquirement and preprocessing

The air-dried soil sample (< 2 mm) was placed in a Petri dish to keep a thickness of approximately 2.0 cm. The VIS-NIR reflectance between 350 and 2500 nm was obtained with a NaturaSpec™ Portable Spectroradiometer (Spectral Evolution, MA, USA) using a contact probe containing an optic fiber and a built-in tungsten halogen light source. Additionally, the VIS-NIR spectrometer was equipped with a silicon photodiode array and a InGaAs photodiode for recording the soil spectral reflectance within the wavelength range of 350–1000 nm and 1000–2500 nm, respectively. The spectrum resolutions were 2.7, 5.5, and 5.8 nm at the wavelengths of 700, 1500, and 2100 nm, respectively, whereas the output spectrum was incremented to the resolution of 1 nm. Furthermore, NaturaSpec™ White Reflectance Plate P/N STDWP-0505 (Spectral Evolution, MA, USA) was applied as the white reference standard material for performing the baseline calibration before and after every 20 spectral measurements. Regarding the heterogeneity of soils, three spectral scans were conducted for each sample.

Compared to absorbance spectra, which require logarithmic transformation and may cause artificial distortions in measurements, reflectance is the directly measured quantity by the applied spectrometer in this study and has been universally regarded as the primary input for soil properties modeling. This is because it preserves the integrity and nature characteristics of spectral data while maintaining the nonlinear relationships inherited from the variation of soil properties, which are crucial for machine learning algorithms [4,19]. Accordingly, the obtained reflectance spectra were directly used in the subsequent data preprocessing. The triplicate spectra reflectance was averaged and trimmed to keep those ranges from 404 nm to 2451 nm for eliminating the edge effects. Moreover, several widely used preprocessing methods, such as first order derivatives, second order derivatives, Savitzky-Golay filtering, wavelets, and standard normal variate (SNV) [20], were tested in the preliminary stage of model development in this study. Among these, SNV, which corrects for single light scattering, generated the best model performance and was therefore selected, aligned with recommendations from previous studies [6,20,21].

The data from 400 samples in the model developing set mentioned in the Soil Characterization section, were randomly split into the calibration data (75% of the data set; $n = 300$) for generating the SOC calibration model and the validation data (25% of the data set; $n = 100$) for examining the model performance (Figure 1). These spectrum preprocessing steps were undertaken in the R studio version 4.1.0 with "prospectr" package [22].

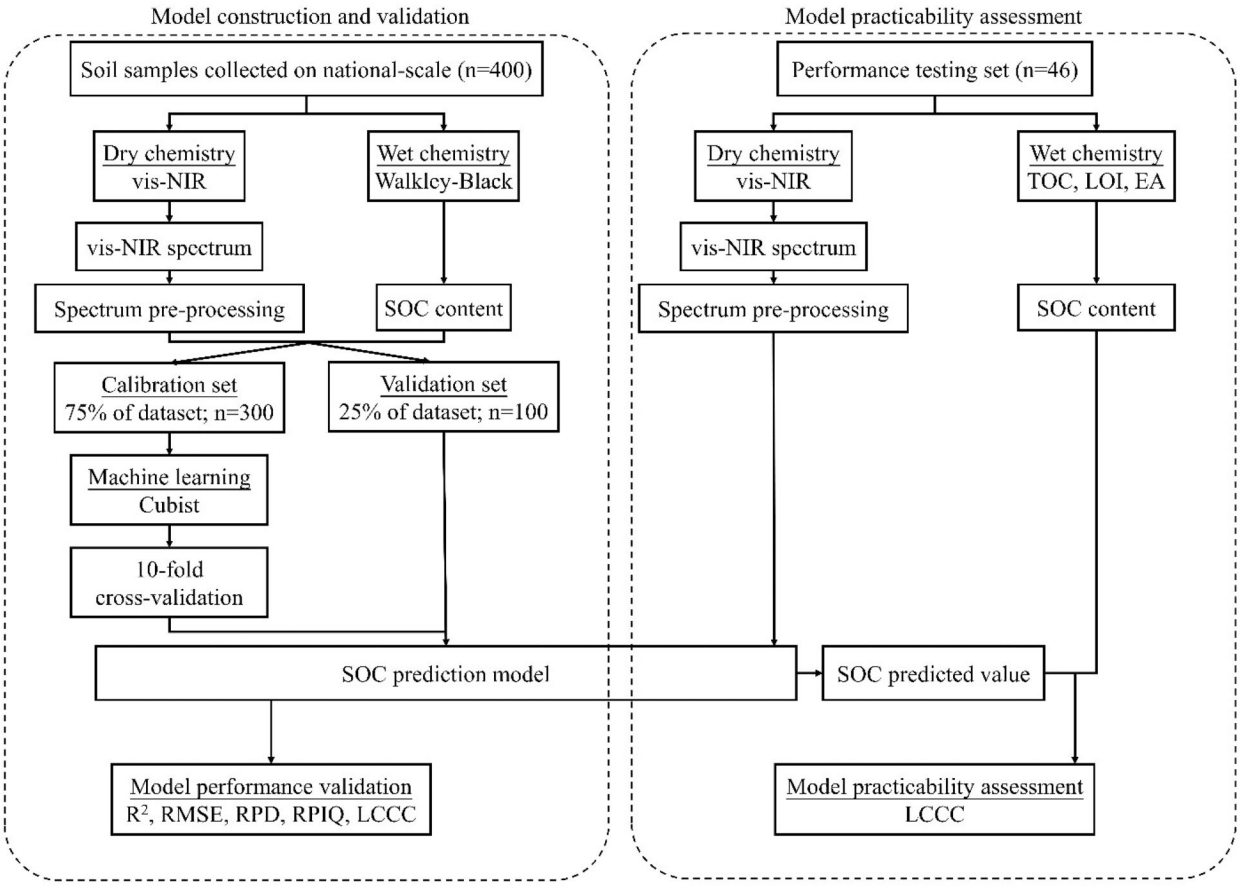

Figure 1. Flowchart for the model construction and practicality assessment. SOC: soil organic carbon; TOC: total organic carbon analyzer method; LOI: loss-in-ignition method; EA: elemental analyzer method; R^2: coefficient of determination; RMSE: root mean square error; RPD: residual prediction deviation; RPIQ: ratio of performance to interquartile range; LCCC: Lin's concordance correlation coefficient.

Calibration model development

Cubist is a rule- and instance-based machine learning algorithm that constructs decision trees, where each terminal node applies a multivariate regression model [8]. This hybrid approach allows to efficiently extract both universal trends of entire dataset and specific relationships shared by certain sub-sample sets, making Cubist especially powerful for coping with the non-linear relationships between SOC content and VIS-NIR spectral reflectance [5]. Moreover, unlike traditional statistical methods, Cubist can model highly context-dependent SOC without using predefined function forms, while generating a more interpretable and well-performing model with a smaller dataset compared than deep learning models [8,9]. Accordingly, the Walkley-Black measured SOC contents and the corresponding preprocessing VIS-NIR spectra from 300 samples in the calibration set, were employed for generating the SOC calibration Cubist model with the "Cubist" package. Herein, for optimizing the input parameters, the model was further tuned over various committees (i.e. 1, 5, and 10) and neighbors (i.e. 0, 1, 2, and, 3) values with 10-fold cross validation using the "Caret" package, which consequently were set to 10 and 2, respectively.

Model performance assessment

The validation set ($n = 100$) were used in the quantification of the model prediction performance for the SOC content. The following statistic measures were employed for the accuracy assessment: the coefficient of determination (R^2), which quantifies the goodness of fitting; the root mean squared error (RMSE), which measures the average error for predicted SOC data comparing to the measured values (Equation 1) [11], the residual prediction deviation (RPD), which evaluates predictive ability relates to the variability of the dataset (Equation 2) [6], the ratio of performance to interquartile distance (RPIQ), which also assesses model performance but is more robust to outliers (Equation 3) [11], and Lin's concordance correlation coefficient (LCCC), which examines the agreement between the predicted and measured SOC contents (Equation 4) [13]:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(x_i - \hat{x}_i)^2}{N}} \quad (1)$$

$$RPD = \frac{SD}{RMSE} \quad (2)$$

$$RPIQ = \frac{IQ}{RMSE} \quad (3)$$

$$LCCC = \frac{2R^2\sigma_x\sigma_{\hat{x}}}{\sigma_x{}^2 + \sigma_{\hat{x}}{}^2 + (\mu_x - \mu_{\hat{x}})^2} \quad (4)$$

where x and $\hat{x}$ stand for the measured and predicted SOC value, respectively; N is the sample size; SD refers to the standard deviation of the measured values; IQ is the range between the upper and lower quartiles; σ implies the corresponding variance; μ is the mean. The RPD value was interpreted as that defined by Chang et al. (2001), that is excellent prediction (RPD $>$ 2.0), moderate prediction (1.4 $\leq$ RPD $\leq$ 2.0), and weak prediction (RPD $<$ 1.4) [23]. As for the other measures, generally, a higher R^2, RPIQ, and LCCC as well as a lower RMSE refer to the better model performance. Additionally, the cross-interactions between the VIS-NIR spectral reflectance within the wavelength range that presented a higher signal-to-noise ratio (i.e. 404 nm to 2451 nm) and the Walkley-Black method measured SOC content as well as the selected soil properties, that directly influenced or varied correspondingly with the SOC content, were quantified with the Pearson's linear correlation coefficient under the significant level of $p < 0.05$. Moreover, to assess the comparability of predictions, the spectra from the model performance testing set were used to generate predicted SOC values, which were then compared with those determined by the TOC, the EA, and the LOI methods. The reliability of prediction was quantified with LCCC (Figure 1). The abovementioned statistical analyses were performed in R version 4.1.0 [22].

Results and discussion

General soil properties and SOC content of the model developing sample set

The soils from a wide range of land uses, geological backgrounds, and soil types contributed the highly diverse soil physical and chemical properties in this study (Table 1). That is, the sand content ranged from 2.40% to 88.8% with a mean and standard deviation of 35.2% and 19.4%, respectively, while the clay content was 0.60–78.3% with an average value of 28.9 ± 17.9% (Figure 2). The pH regime of the studied soil covered that from extremely acidic (pH 2.8) to strongly alkaline (pH 8.5), whereas the average soil pH was 5.5 ± 1.4. Similar to the soil texture and pH, the SOC content of the studied samples ranged widely from 0.04% to 34.7%, while the mean and standard deviation were 2.46% and 3.52%, respectively (Figure 3). Moreover, attributed to the high degradation rate of SOM in humid and tropical regions like Taiwan [24], the SOC content was positively skewed (skewness = 5.6), in which most of the samples owned a SOC level lower than 5%, with a right tailed and leptokurtic distribution (Kurtosis = 40.6).

Cubist model for SOC prediction

Based on the SOC content and the VIS-NIR spectral data from 300 soils in the calibration sample set, the Cubist model achieved an R^2 of 0.94 and RMSE of 1.05% (Figure 4a). While the model performance was excellent (RPD = 3.69), yet the RPIQ was 1.50. Additionally, the model predicted SOC contents highly agreed with those measured by the Walkley-Black method as indicated by the LCCC of 0.96. In terms of the validation set ($n = 100$), which could better represent the model performance. Even though the model expressed a moderate prediction accuracy (RPD = 1.88; Figure 4b), the RPIQ was similar that of the calibration set (1.46). Moreover, a significant linear correlation ($R^2 = 0.72$; $p < 0.05$) and high consistency (LCCC = 0.82) were observed for the SOC contents by the dry lab and wet lab approaches with the RMSE close to that from the calibration data, i.e. 1.09%, suggesting the high reliability of using VIS-NIR spectroscopy for estimating SOC level.

Interactions between model predictors and soil properties

The wavelengths with the model usage over 30%, which were selected to generate the multivariate linear models at the terminal nodes of the Cubist model for the calibration of SOC content, were listed in Table 2. The important predictors at the wavelengths of 1165, 1585, and 1663 nm in the VIS-NIR spectrum stood for the stretching and bending from the organic functional groups with different chemical stabilities, i.e. C-H in the alkyl groups and aromatics as well as C = O in amides (Table 1) [25], which implied the presence of SOM from the various humifaction stages in soils, and thus been identified as reasonable bands for establishing the SOC calibration model using VIS-NIR spectroscopy [19,26].

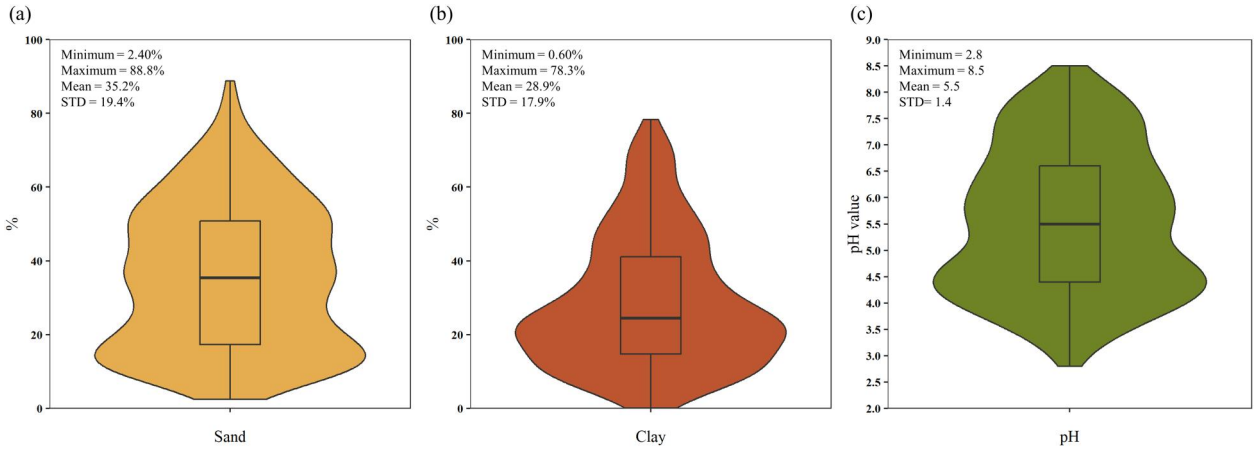

Figure 2. **The violin plot embedded boxplot for the distribution, interquartile range, and median of selected soil properties of the model developing set ($n = 400$). STD: standard deviation.**

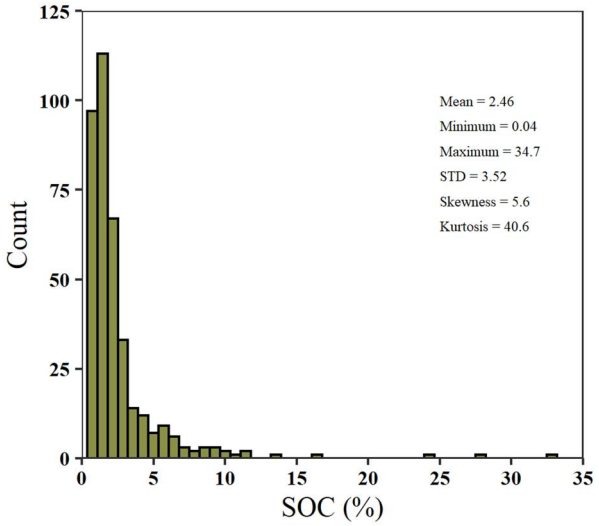

Figure 3. **Frequency distribution of SOC content of the model developing set ($n = 400$). STD: standard deviation.**

Although the prediction model has involved the peaks at 568, 635, and 659 nm which refer to Fe oxides (Table 2) [27], SOM owns an absorption preference at the same wavelength range that could remarkably overwrite the spectrum signature of Fe oxides [28]. On the top of that, owing to the chemical stabilization with the association formations, Fe oxides have been recognized as a carrier for enhancing the degradation resistance of SOM especially in acidic soils [29,30]. The significant ($p < 0.05$) and negative correlations between the SOC content and the reflectance intensity at 500–700 nm (Figure 5), demonstrating the increasing spectral absorption with the increased SOC content. This results numerically illustrated the above-mentioned spectral appearance and soil science observation while supporting the application of characteristic bands of Fe oxides in the constructed Cubist model. Moreover, besides SOC, the negative correlation coefficient was also observed for the reflectance at 500–700 nm with the clay

Table 2. **Important predictors for SOC prediction model.**

Wavelength	Model usage
nm	%
1585	61
568	57
635	49
1383	45
659	33
1379	33
1398	32
1165	32
1663	31
1387	30

content (Figure 5), whereas the spectral features of clay minerals were located at the wave range over 1000 nm [28]. These identical statistical results might be contributed by the co-translocation of secondary minerals (i.e. clays and Fe-oxides) in the humid and tropical soils from Taiwan [24], which led to the similar absorption enhancement with the raising SOC and clay contents.

As for those predictors at approximately 1400 nm, including 1379, 1383, 1387, and 1398 nm (Table 2), the spectral feature was contributed by the hydroxyl group that indicated the dominance of water and clay minerals in the studied soils [27]. Furthermore, the descended reflectance intensity referring to the stronger absorption was found with the enrichment of clay, in which the reduction of SOC was shown (Figure 5). On the other hand, at 2000–2500 nm which is considered as the major fingerprints of clay minerals in a VIS-NIR spectrum [25], this analogous alteration in the reflectance was expectedly observed along with the varied clay content, whilst the positive correlations exhibited between SOC, sand, and pH with the reflectance intensity increase. The spectral pattern differed with the soil properties at around 1400 and above 2000 nm could be considered as a series of consequents from the gradual soil development (Figure 5). Namely, the high temperature

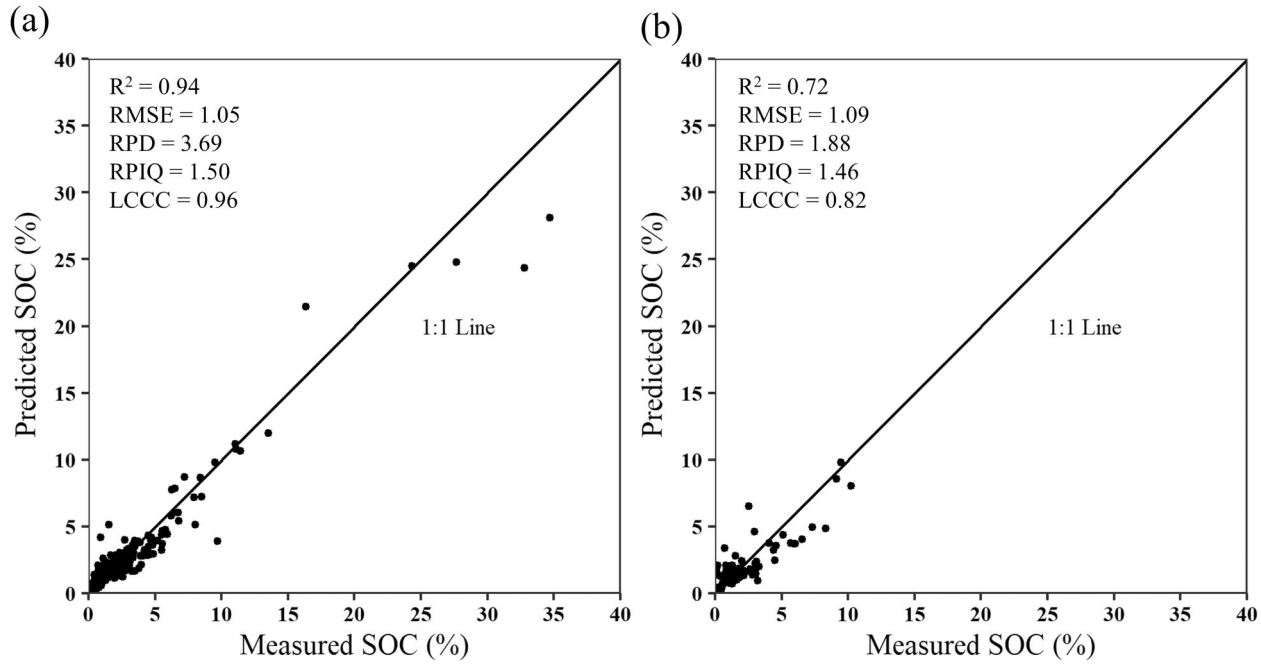

Figure 4. **Relationships between the measured and Walkley-Black method-based Cubist model predicted SOC contents by for calibration set (a) and testing set (b). R^2: coefficient of determination; RMSE: root mean square error; RPD: residual prediction deviation; RPIQ: ratio of performance to interquartile range; LCCC: Lin's concordance correlation coefficient.**

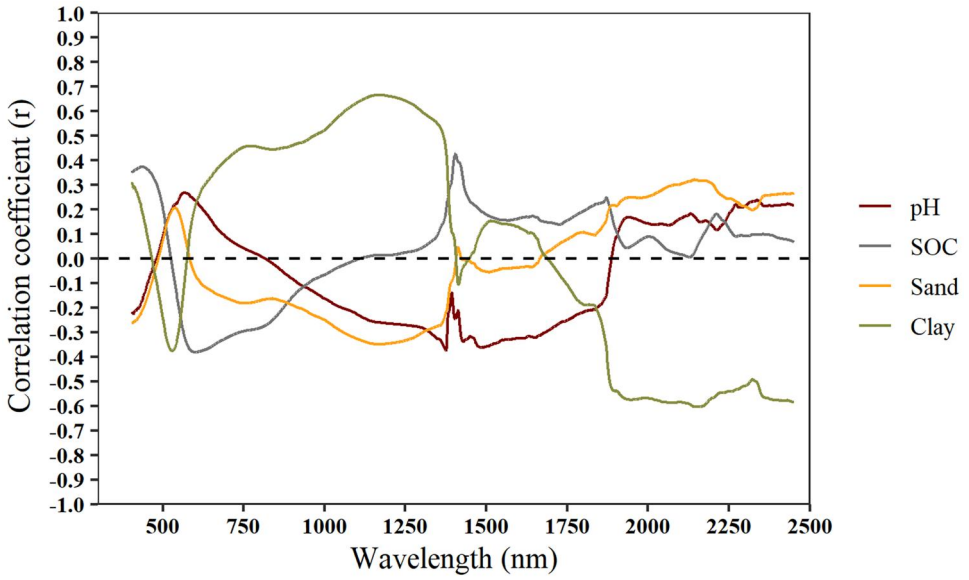

Figure 5. **Pearson correlation coefficients of selected soil properties and VIS-NIR spectral reflectance ($n = 400$). SOC: soil organic carbon.**

and heavy rainfall promoted the decomposition of SOM, which followed by the formation of clay minerals, the breakdown of sand particles, and the enhancement of soil acidity [24]. In other words, the selection of characteristics peaks of clay minerals by the Cubist regression algorithm for the SOC prediction model hinted the influence from the soil weathering on the abundance of SOC (Table 2).

VIS-NIR spectroscopy is characterized by the sensitivity to reflect the highly heterogeneous of soil properties [4], which was contributed by the various soil forming conditions that predominated the SOC abundance, and then gave rise to the statistically diverse VIS-NIR spectrum features. Therefore, the top ten important model predictors in this study constructed a full picture describing the existence and persistence of SOM in the humid tropics (Table 2; Figure 5), and further led to the high SOC prediction precision (Figure 4b), which resembled those reported by Sharififar et al. (2019) for soils from southeast Australia. That is, the peaks referred to the combined effects of SOM and Fe oxides as well as those for the free/lattice water and clay minerals formed a Cubist model with a LCCC of 0.94 [31]. In comparison, the relatively dry

soil condition eliminated the influence from secondary mineral and soil moisture to SOM, and thus only the bands implying the organic groups, i.e. aromatics, phenolics, and methyl groups, were applied in the SOC prediction with the R^2 of 0.85 for soils from northwest China [10].

Model practicality assessment

In the consideration of the adaptability and prevalence of methodologies for SOC determination, different countries/organizations have adopted different wet chemical approaches as the standard methods. For instance, the dry combustion method was applied by U.S. [32] and European Union [33], while the Walkley-Black wet oxidation method was employed by Australia [34] and FAO [35]. In addition to these aforementioned reference methodologies, the LOI method has also been commonly conducted as a simple, rapid, and cost-efficient approach for the SOC determination [3,13,36].

In this study, the SOC prediction model was based solely on the Walkley-Black method (Figure 1). Nevertheless, the predicted SOC contents for the model performance testing set showed significant ($p < 0.001$) and positive correlations with those measured by the TOC and EA methods, both of which are two major branches of the dry combustion approach (Figure 6a, b). Additionally, the predicted SOC values closely aligned with those determined through the wet chemistry, as evidenced by LCCC values of 0.81 for the TOC method and 0.78 for the EA method. This strong concordance was particularly evident in samples with a SOC level below the global average SOC content (3.76%) [37], which represented over 90% of the soils used for model development in this study (Figure 3). However, the deviation between the predicted and measured values slightly increased along the increasing SOC level, which might due to the differences in the mechanisms of the mentioned wet lab approaches (Figure 6a, b). Namely, the small amount of sample weight (usually several milligrams) required by the dry combustion method might introduce the analysis bias due to the high heterogeneous of soils [36]. On the other hand, the existence of Fe/Mn oxides in the studied soils could lead to the extra consumption of the oxidizing agent that causes the overestimation SOC in the Walkley-Black method (Figure 5) [38]. The drawbacks of both wet Walkley-Black oxidation and dry combustion methods possibly provided the uncertainty in the model prediction and SOC evaluation, respectively, which was illustrated by the occasional inconsistency observed (Figure 6a, b). In the case of the LOI method, a positive and significant correlation was also found between the measured and model-predicted SOC contents ($r = 0.71$, $p < 0.001$), whilst the concordance was clearly lower than that of TOC and EA methods as quantified by the LCCC of 0.48 (Figure 6c). The difference was attributed to accounting for the weight loss of the structural water in clay minerals, the presence of which was detected by the variation in reflectance intensity at 1400 nm in the VIS-NIR spectrum (Figure 5), in the LOI method that resulted to the overestimated SOC contents and their dissimilarity with the model predicted values [36].

The considerable prediction precision of the VIS-NIR spectrum-based model in this study was evidenced by the high LCCC values between the predicted SOC values and those measured by the three worldwide prevalent wet lab schemes (Figures 4, and 6a, b). Nevertheless, the common reference methods for SOC determination analyze different carbon-containing components in soils which lead inevitable variation in the outcomes

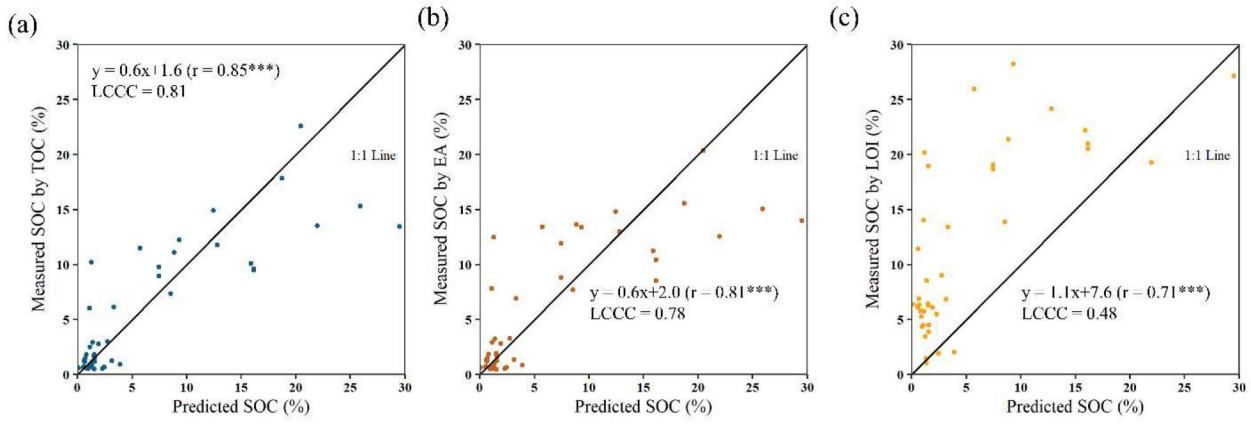

Figure 6. Relationships between the TOC (a), EA (b), and LOI (c) methods measured and Walkley-Black method-based Cubist model predicted SOC contents ($n = 46$). LCCC: Lin's concordance correlation coefficient; ***: $p < 0.001$.

[38]. For instance, the Walkley-Black method was designed for SOC whilst it is incapable for the measurements of recalcitrant SOM (e.g. lignin and phenolic materials) and biochar, which have been considered as the stabilized carbon pool that are the actual contributors for carbon credits [39,40]; the dry combustion and LOI methods target both labile and stabilized carbon in soils, whereas the discrimination between SOC and (bi)carbonates or so-called soil inorganic carbon requires extra sample pretreatments [36]. In comparisons, the model predictors precisely indicated the presence of SOM through the compounds with different turnover rates (i.e. alkyl, aromatics, and amides) and the soil constitutions which (in)directly dominated the decomposition of SOM (i.e. Fe oxides and clays; Table 2), minimizing the uncertainty in evaluating the soil carbon sink and further supported the application of VIS-NIR spectroscopy and the corresponding machine learning model as a sufficient choice for the trustworthy SOC determination under the soil condition in this study.

Conclusions

By evaluating the prediction precision of the VIS-NIR spectroscopy-based Cubist machine learning model for SOC contents against four wet chemistry methods, this study demonstrated that although quantifying SOC through dry chemistry approach unavoidably inherited the analytical uncertainties from the reference data, the strong agreement with universally adopted wet chemistry methods for SOC determination ensured the model's potential for SOC estimation. The developed model incorporated the wavelength regions refer to major SOC components and reflected soil properties known to influence SOC stabilization into the model construction. Given the heterogeneous nature of SOC and the various turnover rates that directly influence the sequestration duration of C in soils, these extracted spectral information further established a scientific foundation of using VIS-NIR spectroscopy for characterizing stabilized soil C sinks. In this context, VIS-NIR spectroscopy serves as a reliable complementary tool to wet chemistry analysis. In the future, with the continued refinement of the model's precision to differentiate between labile and stabilized SOC pools with periodic calibration and validation based on laboratory measurements from various pedoenvironment, this green technology holds promise for evaluating the effects of implementing C-increasing land management practices, thereby improving the adaptation to climate change.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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Data availability statement

The data that support this study will be made available upon reasonable request.

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