Soil organic carbon estimation using VIS–NIR–SWIR spectroscopy: The effect of multiple sensors and scanning conditions

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Abstract

Visible–near infrared–shortwave infrared (VIS–NIR–SWIR) spectroscopy is being increasingly used for soil organic carbon (SOC) assessment. Common practice consists of scanning soil samples using a single spectrometer. Considerations have rarely been documented of the effects of using multiple instruments and scanning conditions on SOC model calibration that occur when merging soil spectral libraries (SSLs), particularly in soils with low SOC concentration and using both field spectroradiometers and laboratory fixed spectrometers. To address this gap, we scanned 143 low-SOC-content soil samples using three spectrometers (ASD FieldSpec 3, ASD FieldSpec 4, and FOSS XDS) and four setup features - FOSS, contact probe (CP), dark-box (DB), and open laboratory (LAB) - at three laboratories. The application of an internal soil standard (ISS) to align one laboratory spectrum with another for spectral correction and spectral merging of various SSLs was examined. SOC models were developed using i) data from each single spectrometer – single laboratory separately and ii) merged data from multiple spectrometers – different laboratories, applying the 1st derivatives of spectra and random forest (RF) regression. The results indicate that the spectral shape and position obtained from all spectrometers and setups did not show any noticeable differences, though spectra based on FOSS setup, particularly on low-SOC samples, demonstrated the highest absolute derivative values regardless of ISS application. The derivative ISS-corrected spectra showed less variation among different spectrometers compared to their uncorrected reflectance spectra. All single spectrometer models predicted SOC reasonably well. However, the spectra acquired by the FOSS setup predicted SOC more accurately ($R^2 = 0.77$ and $SD = 0.04$) than the spectra acquired by the other setups. The models derived from merged uncorrected reflectance spectra yielded poor results ($R^2 = 0.48$ and $SD = 0.10$); nevertheless, assessment of SOC using the 1st derivative ISS-corrected merged SSLs considerably improved the prediction accuracy ($R^2 = 0.70$ and $SD = 0.06$). Hence, the derivative spectra coupled with the ISS correction improved the accuracy of SOC prediction models obtained from merged soil spectra collected in different environments using different instruments. We therefore recommend application of the ISS spectral alignment method linked to the 1st derivative approach to enhance the compilation of SSLs at the regional and global scales for SOC assessment.

Keywords: soil organic carbon, VIS–NIR–SWIR spectroscopy, instrument setup, scanning environment, soil spectral library.

1. Introduction

Soil organic carbon (SOC) plays a fundamental role as an ecosystem indicator and a key parameter of soil quality (Kibblewhite et al., 2008) and soil security (McBratney et al., 2014). Assessment of SOC content has thus drawn considerable attention, in particular for agricultural soils with low concentrations of SOC, where SOC levels risk reaching critical thresholds of, e.g., aggregate stability (Le Bissonnais et al., 1996). As SOC significantly affects the shape and nature of soil reflectance spectra (Gomez et al., 2008) and has strong spectral features (Ben-Dor et al., 1999; Liu et al., 2019), it can be quantified quickly and affordably using visible–near infrared–shortwave infrared (VIS–NIR–SWIR) spectroscopy (Ben-Dor and Banin, 1995; Viscarra Rossel et al., 2019; Gholizadeh et al., 2020).

A major drawback in VIS–NIR–SWIR spectroscopy is that soil spectral information is sensitive to scanning conditions (Ben-Dor et al., 2015), which profoundly influence measured reflectance spectra and the derived models (Ge et al., 2011). Spectra collected in one specific laboratory are, to some extent, influenced by the protocols used, e.g., sampling techniques, sample preparation, temperature, and relative humidity (Pimstein et al., 2011; Chabrillat et al., 2019) or even by scanning habits of different operators (Ge et al., 2011). Here, the term *scanning environment conditions* indicates the abovementioned factors. Spectral performance and model accuracy may vary significantly among different types of spectrometers or even among models from the same manufacturer (Pimstein et al., 2011) due to equipment specification and setup, measurement repeatability, geometry during spectral acquisition, calibration and performance of sensors, efficiency of optical fibers, illumination source, and viewing angles of measurements (Ge et al., 2011). We use the term *instrument conditions* to collectively refer to these factors.

Consequently, choosing the appropriate instrument and environment conditions is crucial for effective soil spectra investigation; it is equally important to analyze, evaluate, and interpret the

72 outputs. Different spectrometers such as ASD FieldSpec (Ben-Dor and Banin, 1995; Gholizadeh
73 et al., 2018b), PSR+ Spectral Evolution (Tsakiridis et al., 2017; Tzios et al., 2019), and FOSS XDS
74 (Genot et al., 2011; Stevens et al., 2013; Castaldi et al., 2018) were globally used to develop SOC
75 prediction models. Apart from the instrument, various analytical methods are used, which can also
76 significantly influence the prediction performance of the spectroscopic models and hence hinder
77 the exchange of SOC data between laboratories. If soil spectral libraries (SSLs), consisting of
78 thousands of soil samples, need to be merged, managing the large variation resulting from different
79 scanning environments and instrument conditions remains a challenging task. Given this issue,
80 other communities (e.g., food and fodder quality control) have developed a set of standard samples
81 to enable the exchange of data and models between scanning environments and instruments (Shenk
82 et al., 2001; Fearn, 2001; Ge et al., 2011). In the soil spectroscopy community, this issue has
83 recently been raised and only a few authors have started developing standards and protocols
84 including proposals for fixed geometry and spectral preprocessing (e.g. Ben-Dor et al., 2015);
85 however, it is still a matter of intense debate.

86 Knadel et al. (2013) used three VIS–NIR–SWIR spectrometers with varying resolutions and
87 spectral ranges under uniform laboratory conditions for SOC assessment to compare the
88 performance of each single instrument, albeit without transferring the prediction models from one
89 instrument to another. Ge et al. (2011) compared different VIS–NIR–SWIR spectrometers under
90 different conditions for predicting SOC in the same population of soil samples with the same
91 treatment (sampling technique, sample preparation, and sample roughness) applying the same
92 analysis technique (preprocessing, calibration, and validation). They used three calibration transfer
93 methods (slope and bias correction, direct standardization, and piecewise direct standardization) to
94 transfer calibration models from one instrument to another. Pimstein et al. (2011) minimized the
95 effects of different scanning environment and instrument conditions by developing a standard

protocol and the internal soil standard (ISS) concept. This concept is a simple realignment procedure adopting an agreed-upon reference material that can be used to align one spectrum (under any condition and setup) to another. It offers the possibility to align spectra from different origins and merge them in a single SSL. Ben-Dor et al. (2015) introduced two sand dune samples from the southwest coast of Australia as ISS samples, named from their location of origin as Lucky Bay (LB) and Wylie Bay (WB). They were examined by various users (Ben-Dor et al., 2015; Romero et al., 2018; Chabrillat et al., 2019; Crucil et al., 2019) to check their robustness for alignment of the spectra obtained from different instruments. Generally, the LB (99% quartz) provided better results. Nevertheless, its capability to improve SOC prediction has only been tested by Crucil et al. (2019), who trained SOC models using soil spectra acquired in laboratory conditions for outdoor spectra with the alignment by the LB internal soil standard.

Given the importance of SOC assessment for agricultural soils with low SOC content, as well as the effects of scanning environment and instrument conditions on the final performance of soil prediction models, the current study was conducted under four different setups at three different laboratories: the Czech University of Life Sciences Prague (CZU), the German Research Center for Geosciences (GFZ), and the University Catholique de Louvain (UCLouvain) with the aims of i) comparing the low-SOC-content soil spectra measured with different spectrometers under different scanning environment conditions, ii) examining the potential of three VIS–NIR–SWIR spectrometers (ASD FieldSpec 3, ASD FieldSpec 4, and FOSS XDS) under four different setups and different three laboratories to develop SOC models for agricultural soils of the Czech Republic, and iii) assessing the potential of the ISS approach (LB sample) linked with common spectral preprocessing to improve the predictability of SOC models derived from merged SSLs.

The results contribute to implementing a rapid and low-cost procedure for SOC analysis, particularly in agricultural soils with low SOC content, choosing a mature technique and a satisfactory measurement protocol with appropriate performance.

2. Materials and methods

2.1. Study sites

Three typical agricultural sites with low SOC content from different parts of the Czech Republic were chosen (Figure 1): Vidim ($50^{\circ}46'0''$ N, $14^{\circ}51'0''$ E, area 7 ha, altitude 315–323 m above sea level (a.s.l.), average annual temperature $7-8^{\circ}\text{C}$, average precipitation 550–650 mm), Sedlčany ($46^{\circ}68'0''$ N, $14^{\circ}42'0''$ E, area 5 ha, altitude 375–387 m a.s.l., average annual temperature $7-8^{\circ}\text{C}$, average precipitation 550–650 mm), and Brumovice ($48^{\circ}96'0''$ N, $16^{\circ}88'0''$ E, area 4 ha, altitude 187–227 m a.s.l., average annual temperature $9-10^{\circ}\text{C}$, average precipitation 550–650 mm).

Figure 1. The Czech Republic and location of the study sites in the country.

According to the World reference base for soil resources (WRB, 2014), the original soil type in Brumovice was a Haplic Chernozem on loess that transformed over time to a Regosol (steep parts) and Colluvial soil (foot slope and the tributary valley) due to erosion and sedimentation. For Vidim,

the original soil type was a Haplic Luvisol on loess, and for Sedlčany a Haplic Cambisol on gneiss. A similar process of soil degradation resulting in a change of soil type can be detected at these sites as well.

2.2. Soil sampling and measurements

We collected 143 soil samples from the topsoil (0–20 cm) within regular grids covering the sites (Figure 2). Regarding field size, soil conditions, and selected sampling and analyzing algorithms (Kuang and Mouazen, 2012; Ramirez-Lopez et al., 2014), the sample size had adequate coverage of the predictor space and it was representative of the population to which the models were applied. The position of each sampling point was recorded using a GeoXM (Trimble Inc., Sunnyvale, CA, USA) receiver with accuracy of 1 m.

Figure 2. Location of sampling points.

The soil samples were air-dried, sieved to ≤ 2 mm, and thoroughly mixed before analysis (ISO11464:2006). SOC was measured as total oxidized carbon (Table 1) using wet oxidation (ISO 14235:1998).

Table 1. Statistical summary of SOC data

Parameter	SOC (%)
Mean	1.28
Median	1.17
Minimum	0.62
Maximum	2.74
SD	0.2
CV	16

SD: standard deviation; CV: coefficient of variation

2.3. VIS–NIR–SWIR spectroscopic measurements

Spectroscopic measurements were recorded in the VIS–NIR–SWIR range (400–2500 nm) at the CZU, the GFZ, and the REQUASUD agricultural extension service network laboratories (commissioned by the UCLouvain), using three different spectrometers: ASD FieldSpec 3 Pro FR (ASD Inc., Denver, CO, USA), ASD FieldSpec 4 Pro FR (ASD Inc., Denver, CO, USA), and XDS Rapid Content Analyzer (FOSS NIR Systems Inc., Laurel, MD, USA) (Table 2).

Table 2. Instruments specifications

Spectrometer	Wavelength range	Spectral resolution	Spectral interval
ASD FieldSpec 3 Pro FR	350–2500 nm	3 nm @ 350–1050 nm	1.4 nm @ 350–1000 nm
		10 nm @ 1051–2500 nm	2 nm @ 1001–2500 nm
ASD FieldSpec 4 Pro FR	350–2500 nm	3 nm @ 350–1050 nm	1.4 nm @ 350–1000 nm
		10 nm @ 1051–2500 nm	2 nm @ 1001–2500 nm
FOSS XDS Rapid Content Analyzer	400–2498 nm	0.5 nm	2 nm

All instruments were operated under the routine protocols and conditions of their respective labs; some external factors such as temperature (20–23 °C) and relative humidity (40–45%) were almost similar. The ASD FieldSpec spectrometers measure using a Si Photodiode and an InGaAs SWIR detector. Their spectral resolution is 3 nm for the 350–1050 nm region and 10 nm for the 1051–2500 nm region. ASD FieldSpec 3 and ASD FieldSpec 4 provide a spectral sampling of 1.4 nm in the 350–1000 nm spectral range and 2 nm in the 1001–2500 nm spectral range, although data are interpolated to 1 nm intervals. The FOSS XDS spectrometer measures the reflectance continuously in the 400–1300 nm region with a Si detector and 1300–2498 nm with a Pbs detector, offering a

spectral resolution of 0.5 nm (4200 wavelengths). Measurements using ASD FieldSpec 4 at the GFZ were recorded under two different setups: the common setup and a dark-box (DB) environment developed at the GFZ. The details of each measurement protocol are presented in the following sections.

2.3.1. Measurements at the CZU

For the spectra measurements by ASD FieldSpec 3 at the CZU, a high-intensity contact probe (CP), powered by a 6.5W tungsten-quartz-halogen lamp, was chosen (Figure 3). Here, we introduce this setup as CP.

Figure 3. Measurement setup at the CZU (CP).

The instrument ran for 30 minutes to warm up the spectrometer and lamp. The soil samples were placed in 5 cm diameter petri dishes and levelled with a stainless-steel blade (formed a 2 cm layer of soil) to guarantee a flat surface flush with the top of the petri dish as a smooth soil surface ensures maximum light reflection and a high signal-to-noise ratio (SNR) (Mouazen et al., 2005). The samples were lifted up to the CP assembly by a manual elevator and all spectral readings were recorded in the center of the samples (three replications each). The spectrometer was calibrated prior to the first and after every 10 measurements using a white SpectralonTM panel (Labsphere,

North Sutton, NH, USA) and prior to the first and after every 5 measurements using the LB sample (Ben-Dor et al., 2015).

2.3.2. Measurements at the GFZ

At the GFZ, two series of spectra measurements, both using ASD FieldSpec 4, were recorded under the common (LAB) and DB setups (Figure 4). Soil samples for spectra measurements were prepared in the same way as at the CZU (Section 2.3.1.).

Figure 4. Measurement setups at the GFZ: LAB (left) and DB (right).

The spectral measurements under LAB setup were performed using an ASD Lamp Pro as the light source. Artificial light was installed at an $\sim 35^\circ$ zenith viewing angle and the instrument warmed up for 60 minutes before the actual scanning. The samples were located ~ 7 cm in nadir below and in the middle of 8° opening angle fore-optics and measured in the center of the samples (three replications each, rotating and steering the sample, flattening before each measurement) in a dark room to avoid interference from stray light. The spectrometer was optimized using a SpectralonTM white reference (Labsphere, North Sutton, NH, USA) at the beginning and end of each batch of 5 soil sample measurements. The LB sample was scanned after the SpectralonTM white reference at the beginning of each batch and before the next SpectralonTM measurement at the end of each batch.

The DB was developed at the GFZ (Figure 5) following the concept reported by Ben-Dor et al. (2015). The objective of the design was providing a measurement setup with fixed geometry for lighting and variable samples. The distance of different objects to the sensor should be feasible and samples can be rotated for taking multiple measurements. To exclude stray light from random light sources, a wooden box was built; reflection the inside was further reduced by applying black paint to the inside of the box. To reduce shading on uneven samples, two halogen bulbs were used for illumination, both are pointing at 45° downward at the sample. The selected bulbs had to be without a front/diffusor window to avoid adding spectral transmission features. The lamps were powered by a switching power supply and an uninterruptible power source (UPS) to avoid interference artifacts due to voltage oscillations. The ASD fiber optics were mounted above the center of the rotary table and different fore-optics can be attached to the mount.

Figure 5. Photograph (left) and schematic (right) of the dark-box developed at the GFZ.

The spectra measurements under the DB setup were acquired with an 8° fore-optic and a nadir viewing sensor ~ 7 cm above the target, producing a ~ 1 cm ground instantaneous field of view (GIFOV) in the middle of the sample. The same batch procedure was used as for the LAB setup with three replication measurements (rotating and steering the sample, flattening before each

measurement), optimization using a SpectralonTM white reference (Labsphere, North Sutton, NH, USA), and acquisition of the LB sample measurements at the beginning and end of each batch of 5 soil samples.

2.3.3. Measurements at REQUASUD commissioned by the UCLouvain

For soil spectra measurement using the FOSS XDS spectrometer (termed FOSS setup in this paper), the samples were sent to Province of Liege Laboratories (member of the REQUASUD network). According to the standard protocol of the REQUASUD laboratories for soil scanning (Genot et al., 2011), two quarter cups were filled with soil material (~25 g) for each soil sample. Thus, the soil samples were measured in duplicate, and for each subsample, an averaged absorbance spectrum was obtained from 32 scans. The spectra averaged between the two subsamples were recorded if the root mean square error (RMSE) between the two spectra of each subsample was close enough based on a t-student test conducted with previously scanned samples; otherwise, the average spectrum was discarded and the sample was scanned again using the same procedure described above. The LB sand was scanned, following this procedure, every 20 soil samples.

2.4. Spectral preprocessing, modelling, and evaluation

Before using the data in SOC models, spectral data obtained from all setups i) at each single laboratory by each single spectrometer separately and ii) at different laboratories by multiple spectrometers were preprocessed.

2.4.1. Single spectrometer – single laboratory

For single laboratory modelling, the three replicates measurements were averaged. The noisy portions between 350–399 nm and 2490–2500 nm (for ASD FieldSpec spectrometers) and 400–447 nm (for FOSS XDS spectrometer) were removed and the reflectance spectra were subjected to Savitzky-Golay smoothing with a second-order polynomial fit and 15 smoothing points to remove the artificial noise caused by the spectrometer (Ren et al., 2009; Song et al., 2012). Then, the 1st derivative transformation was used as a spectral preprocessing algorithm. This is effective for removing baseline offset and according to some researchers, produces the best results and higher accuracy among the other techniques for developing soil spectral models (Duckworth, 2004; Bendor et al., 2008; Gholizadeh et al., 2015).

The datasets were divided into calibration (75% of samples) and validation (25% of samples) sets using 100 times random stratified sampling (Gholizadeh et al., 2018a). For modelling, the ensemble machine learning algorithm random forest (RF) regression was used (Breiman, 2001). RF works by growing a group of regression trees based on binary recursive partitioning, where the feature space is repeatedly split into regions involving observations with similar response values (Strobl et al., 2009). It minimizes the risk of overfitting and using it almost no fine-tuning of parameters is needed to produce good predictions (Diaz-Uriarte and Andres, 2006; Saberioon et al., 2018). To assess the model performance, standard model evaluation statistics: the coefficient of determination (R^2) between the observed and predicted values of SOC and standard deviation (SD) were used, which were averaged for 100 repetitions in the validation set to quantify the validation accuracy every time. Fisher's least significant difference (LSD) test was then applied to evaluate the statistical differences to verify the existence of a significance difference in case of model accuracy (Castaldi et al., 2016).

2.4.2. Multiple spectrometers – different laboratories

For inter-laboratory modelling, the preprocessing procedure was conducted by applying the same method as for each single laboratory (section 2.4.1.). However, to remove noise and non-linearity effects, wavelengths were cut off to 448–2488 nm. In addition, the ASD FieldSpec spectrometers data were resampled to the 0.5 nm spectral resolution of the FOSS XDS spectrometer. In addition, before transformation of the spectra to the 1st derivative, the spectra were corrected by the ISS standard. Following the suggestion of Pimstein et al. (2011) adopted by Ben-Dor et al. (2015), a correction factor (CF) was used in the ISS realignment procedure to align all setups. The reflectance value of each sample acquired from the different setups was corrected multiplying the CF with the original spectrum. The details of the CF and its implementation for spectral correction were previously described by Ben-Dor et al. (2015) and Chabrillat et al. (2019). Afterward, the model derived from the LB-corrected spectra of all laboratories and multiple spectrometers was developed. The random stratified sampling was used 100 times to provide the calibration set (75% of samples) equally distributed in all laboratories (full range selection in each laboratory). Similar to the procedure used for single laboratories, RF was used for spectral modelling of SOC using the merged data of all laboratories. The final prediction accuracy was assessed using R^2 and SD. These metrics were averaged for 100 repetitions in validation set equally distributed over all laboratories (full range selection in each laboratory).

3. Results and discussion

3.1. Soil spectral features assessment

The mean 1st derivative LB-corrected spectra of all samples with different range of SOC contents (lower contents: 0.62–0.75% and higher contents: 2.02–2.74%) scanned at three laboratories by three different spectrometers (under four different setups) are shown in Figure 6. They were also

compared with the uncorrected reflectance spectra, which are the most commonly used spectra in VIS–NIR–SWIR spectroscopy (as a reference).

Figure 6. Mean spectra of samples with lower (left) and higher (right) range of SOC contents measured by the FOSS, CP, DB, and LAB setups at different laboratories: uncorrected reflectance spectra (top) and 1st derivative LB-corrected spectra (bottom).

There were no significant changes in spectral features and the general shape of the curves remained constant under all scanning environments and instrument conditions within both uncorrected reflectance and 1st derivative LB-corrected spectra categories and in both SOC ranges (Figure 6). Several absorption features, including features of Fe oxides in the VIS range (400–700 nm) were obvious in all spectra (particularly in derivative spectra) regardless of the SOC content ranges, instruments, and laboratories. The absorption features of O–H bands at 1400 nm and 1900 nm, and

a doublet around 2200 nm related to the O–H of hygroscopic water and clay minerals lattice (Ben-Dor et al., 1999) were clearly observed. The curve and spectral features are similar to those described by Ge et al. (2011) and Knadel et al. (2013) using multiple spectrometers, and Romero et al. (2018) using ISS correction.

Figure 6 also highlights that despite the spectra's similar shape and spectral features position in each group, the absorption intensities of spectra varied, mainly in the VIS range (as SOC is more active in this region) of low-SOC samples depending on the spectrometer used. The differences among spectra in absorption/reflectance intensities in the NIR and SWIR regions were smaller in both reflectance and derivative spectra. The FOSS spectra, specifically for low-SOC samples, had the highest absolute derivative values/the lowest reflectance values at almost all wavelengths regardless of the preprocessing approach and LB application. This is probably due to the short distance between the sample, light source, and the more controlled environment within the FOSS setup. In a study by Romero et al. (2018), evaluating the effect of spectrometers' light source distance to soil sample, the spectra derived from a CP setup with shorter target and illumination distance showed higher values across the entire spectrum. They mentioned that the distance between the light source and the target significantly influences the reflectance intensity of soil samples. Hence, variation between sensors measuring the same soil samples may be caused by noise during acquisition, integrity of the optical fibers, illumination variation, and the performance of each detector in each spectral region (Pimstein et al., 2011). The same results were obtained by Ge et al. (2011) and Chabrillat et al. (2019) measuring the same samples under various sensor setups.

The uncorrected spectra (Figure 6, top) indicated that there were stronger variations among the spectra, (particularly for low SOC contents) obtained from different spectrometers, setups, and laboratories. These differences decreased after LB correction (Figure 6, bottom). This

demonstrated the capability of the LB sample to minimize the existing systematic variations among different scanning instruments and environment conditions. The methodology narrowed the deviation of soil spectra (for the same samples) and reduced the differences between sensors and laboratories, which was also reported by Gholizadeh et al. (2017) and Romero et al. (2018).

3.2. Single spectrometer – single laboratory models for SOC prediction

According to Ben-Dor et al. (2015), the ISS spectral realignment procedure improves SOC prediction when models are calibrated using spectra from different sources. In order to show the differences between different laboratories and measurement conditions and for development of the SOC prediction models at each single laboratory (CZU, GFZ, and UCLouvain) using the spectrum from each individual spectrometer setup (FOSS, CP, DB, and LAB), the 1st derivative spectral information without LB correction was used (Figure 7).

Figure 7. SOC prediction using single FOSS, CP, DB, and LAB spectrum obtained at UCLouvain, CZU and GFZ laboratories. The red line indicates the averaged R^2 for 100 validation splits (25%).

The model developed for SOC using the FOSS setup performed best with a R^2 of 0.77 and SD of 0.04 followed by the CP with R^2 of 0.74 and SD of 0.05. Both models are classified as having good prediction accuracy (Chang et al., 2001). The LSD test carried out on the validation statistics of all datasets also confirmed that the FOSS data provided significantly better estimation accuracy compared to other instruments and setups (Table 3). The LAB setup, using ASD FieldSpec 4 Pro FR in open laboratory conditions, had the lowest R^2 (0.64) and the highest SD (0.09) in validation performance, although according to Chang et al. (2001), these results are still fair ($0.5 \leq R^2 \leq 0.7$). The results of the SOC estimation produced by the DB configuration showed similar SD values of 0.05 to the CP-derived model. The model derived from spectra measured with a CP yielded a higher R^2 of 0.74. In addition, the LSD test detected a significant difference between DB and CP setups for SOC assessment (Table 3).

Table 3. Least significant difference test

Setup	R^2	Group
FOSS	0.77	a
CP	0.74	b
DB	0.70	c
LAB	0.64	d

Spectrometers are governed by the instrument's stability, SNR, configuration, illumination source, detector performance, fore-optic and fiber optic characteristics, stray light contribution, and warm-up time (Ben-Dor et al., 2015). Therefore, the variation in modelling accuracy can be expected. These differences can also be considered as the expected errors in routine standards applied in the laboratories and even operators' measurement habits (Genot et al., 2011; Pimstein et al., 2011). In contrast, Knadel et al. (2013) and Romero et al. (2018) found no variation in clay modeling performance between three different field spectrometers. The best performance using the FOSS XDS can be explained by its particular advantages of a closed environment, fixed light sources,

and stability of the probe measurements, which reduce the possibility of error. Regarding the CP setup, acceptable results were obtained that can be attributed to the use of a mechanical stand for holding the contact probe, decreasing the vibrations compared to a handheld setup (Pimstein et al., 2011). The lower predictive power of the LAB setup is probably caused by stray light that can be connected to the single light source and distance between object and light source (Ge et al., 2011).

3.3. Multiple spectrometers – inter laboratory models for SOC prediction

For inter-laboratory modelling, the datasets obtained from each spectrometer at each laboratory were merged to develop a single SOC model. For calibration of the models, the LB correction was first applied on the reflectance spectra. The spectra were then transformed to Savitzky-Golay + 1st derivative spectra. The model was compared with the models obtained from merged uncorrected reflectance spectra as a reference (Figure 8).

Figure 8. SOC prediction using FOSS-CP-DB-LAB merged spectra obtained at different laboratories with (top) and without LB correction (bottom). The red line indicates the averaged R^2 for 100 validation splits (25%).

The predicted SOC from the uncorrected reflectance spectra presented an obvious wider scattering with low accuracy and poor performance ($R^2 = 0.48$ and $SD = 0.10$). R^2 was considerable higher

value ($R^2 = 0.70$) and SD showed a lower value (0.06), when using derivative spectra coupled with the LB correction in comparison with uncorrected reflectance spectra. The ISS correction (LB) improved the prediction accuracy of SOC using reflectance spectra due to the capability of the LB sample to align the spectra acquired in different laboratories and using multiple spectrometers (Ben-Dor et al., 2015). Generally, the optimal case was combining the derivative spectra and LB standard to increase inter-laboratory comparability. The suitability of this approach and derivative spectra agrees with the results reported by Pimstein et al. (2011), who confirmed a better performance of using the derivatives coupled with ISS correction compared to using raw reflectance spectra.

The SOC models calibrated on the merged SSLs were slightly less accurate compared to most of the single models that were calibrated on a single instrument in a single laboratory (Figures 7 and 8). This can be expected as, by combining datasets, we introduce more sources of variation as a result of different scanning environments and instrument conditions (Ge et al., 2011). It can also be explained that if a strict protocol (geometry, spectrometer, environmental condition, and users) is used, even without correction, the prediction performance would be reliable as a result of the smaller systematic errors by applying a precise protocol (Romero et al., 2018). Nonetheless, merging SSLs using spectral derivatives and standards such as ISS correction (the LB sample in this study) can lead to the development of a regional/global calibration model that extends the applicability of the model at the cost of a small reduction in prediction accuracy. This is particularly important considering the recent developments such as the European Land Use/Cover Area Survey (LUCAS) SSL that could be spiked or merged with local SSLs from different research institutes (Orgiazzi et al., 2018).

Notably, here, we dealt with three spectrometers, four setup features and three laboratories, as well as the same soil sample set. However, for development of a large-scale SSL with diverse soil

samples and scanning conditions, the promising role of the ISS approach linked to spectral preprocessing techniques in providing acceptable prediction accuracies is more evident (Ben-Dor et al., 2015; Chabrillat et al., 2019). In this case, a more significant improvement of the model performance can be observed.

Conclusions

Based on the spectral analyses of 143 agricultural soil samples with a low SOC content, the spectral shape and position obtained from different spectrometers and setups (FOSS, CP, DB, and LAB) did not show any noticeable differences, but there was a variation in the absorption intensities of spectra acquired by the spectrometers, particularly in the VIS range. The spectra based on the FOSS setup yielded the highest absolute derivative values/the lowest reflectance values at almost all wavelengths. The derivative spectra corrected with the LB standard indicated less variation among different spectrometers' spectra compared to their uncorrected reflectance spectra. The results also highlighted that despite the fair to good calibration accuracy of all single models, the derivative spectra obtained from the FOSS XDS spectrometer, which scans under more stable and controlled conditions, produced in a more reliable SOC prediction model compared to other spectrometers, which was confirmed by the LSD test. When the reflectance spectra from multiple spectrometers and laboratories were merged, the outputs were poor, although the 1st derivative LB-corrected spectra of soil mixed from different scanning environments and instrument conditions significantly improved the model accuracy. In this case, the findings showed that the sets of derivative spectra matched remarkably with the LB correction minimizing those variations enabling the merging data process, which is an essential part of establishing any SSL. Nowadays, when users are sharing data derived from diverse soil samples, different scanning environments, and various instruments for building SSLs and developing regional/global models; the use of standards (e.g., the LB approach)

for reducing the variation and better merging of soil spectral databases is recommended. This allows direct comparison and use in quantitative models of spectra acquired in diverse conditions. In this study, we focused only on SOC (mainly low contents) in one set of soil samples; however, other soil properties and several soil datasets still need further investigation.

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