

ASSESSING THE UTILITY OF THE VISNIR-MOUNTED PENETROMETER

A Thesis

by

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ABSTRACT

Proximal soil sensors, such as a VisNIR spectrometer mounted into a penetrometer, are being developed as tools to measure soil properties *in situ* with the goal of providing real-time and spatially explicit soil characterization and measurements without traditional laboratory data. This work addresses major challenges and questions facing the implementation of this technology as it gains popularity for commercial use. Research seeks to determine 1) whether external parameter orthogonalization (EPO) is a robust method to remove soil moisture effects from *in situ* spectra, 2) if there is an influence of library and EPO dataset on soil property predictions such as clay and organic carbon content, 3) if spectra should be averaged (e.g. by depth or by horizon), 4) if VisNIR spectroscopy is better at predicting surface versus subsurface soil properties, and 5) whether spectral predictions of soil properties, such as clay content, are helpful to classify soils. To assess the modeling decisions on clay and carbon content predictions, three dried ground soil spectral libraries were calibrated and transformed with three EPO datasets to predict Illinois soils. Results indicated that both Texas state and national libraries could provide robust soil property predictions with the Texas EPO. A second experiment implemented spectral averaging and soil prediction averaging in two model scenarios (using an intact, field moist library or a dried ground library and EPO) and reported that averaging may provide a slight increase in prediction accuracy, and supported the notion that a dried ground library and EPO is a robust way to predict soil properties and that subsurface soils produce more accurate clay content predictions than

surface soils. VisNIR predictions of clay content were able to categorize soils into series more precisely than soil mapping. Further research may consider real-time characterization and further support is also needed to assess the prediction differences in surface and subsurface soils and the driving influences.

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NOMENCLATURE

EPO	External parameter orthogonalization
SOC	Soil organic carbon
PLS	Partial least squares
RMSE	Root mean squared error
VisNIR	Visible near-infrared

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1. INTRODUCTION

Reliable remote and proximal soil sensors are needed for improved resolution soil mapping and tracking long-term management changes (Wenjun et al., 2019; Adamchuk et al., 2004). Scientists can use estimates of clay content, moisture, C content, and bulk density to predict the impact of land management on soil health. Scientists often rely on proximal and remote soil sensors for this information due to their speed, low cost (relative to traditional chemical analyses), and most importantly, their ability provide quantitative estimates of soil properties across large areas (>100 ha) and over time (Viscarra Rossel et al., 2011).

There are several widely-used and commercially-available remote and proximal soil sensors that can collect spatial information both horizontally (across the soil surface) and vertically (diving into the soil profile). Many sensors provide high resolution data across a landscape, but low vertical quality soil data. For example, electromagnetic induction, and electrical conductivity devices, such as an EM38; DueEM, and Veris, provide outstanding information on where soils change across a landscape. These sensors integrate soil information to a depth of 1 to 2 m; however, interpreting the information vertically is less straightforward. The bulk electrical conductivity integrates soil water, clay, and salinity properties at depth (Geonics Ltd., Mississauga, ON, Canada).

In summary, proximal sensing with bulk soil electrical conductivity still requires probing the soil profile with traditional soil sampling equipment (Adamchuk et al.,

2017). Other types of sensing, such as passive gamma sensing, have the same limitation (Rouze et al., 2017). Remote sensing only views the soil surface or a shallow layer of less than 10 cm thickness (Ben-Dor et al., 2009). VisNIR spectroscopy, although traditionally employed in the laboratory, is one of few technologies capable of being employed for fine-resolution vertical soil sensing (Viscarra Rossel et al., 2011).

1.1. VisNIR Spectroscopy for Soil Science

VisNIR spectroscopy is a sensing technology that can rapidly and non-destructively characterize soils (Ben-Dor and Banin, 1995, O'Rourke and Holden, 2011). Perhaps the most useful feature is that multiple properties can be detected from the same dataset (Brown et al., 2006; Viscarra Rossel et al., 2006; Poggio et al., 2015; and Soriano-Disla et al., 2014). The visible (400-700 nm) and near-infrared (700-2500 nm) wavelength regions contain information about the presence and abundance of chromophores, chemical components in the soil that interact in this region of the electromagnetic spectrum (Ben-Dor et al., 1999).

Chromophore information appears as absorption features in VisNIR spectra (Ben-Dor et al., 1997). Some examples include OH in free water, clay mineral lattices, organic matter, and other features such as iron oxides, salts, or carbonates (Ben-Dor et al., 1999). In the NIR region, specifically, one can find overtones of O-H and H-O-H vibrations of free water at ~1.455 and 1.915 μm in addition to the O-H stretching and metal-OH bends and vibrations in soil clay lattices at 1.415 and 2.207 μm (Ben-Dor et al., 1997). Physical soil properties may also affect the soil VisNIR spectra. Particle size

distribution and aggregation can adjust baseline height and overall absorption of the spectral curve through light scattering or reflection (Ben-Dor et al., 1999).

The most common application of VisNIR spectroscopy to soil science is predicting clay, organic C, and related properties (e.g., total nitrogen and cation exchange capacity) from dried ground soil spectra. Several soil spectral libraries of sieved and dried soil samples exist (Waiser et al., 2007; Brown et al., 2007; Wijewardane et al., 2020). The USDA-NRCS Kellogg Lab spectral library is particularly useful because it is publicly accessible, quite large (~20,000 samples and growing), and covers many soils across the USA. These libraries list the soil spectra at 10 nm increments from 500 to 2450 nm along with full or partial soil characterization. Most common soil characteristics in soil spectral libraries include sand, silt, clay, total C, and carbonate content, as well as pH and cation exchange capacity (Chang et al., 2001; Shepherd and Walsh 2002; McCarty et al., 2002).

Recent *in situ* VisNIR development has progressed towards creating a penetrometer-mounted VisNIR spectroscopy for the real-time prediction of soil properties (Ackerson et al., 2017; Wijewardane et al., 2020). With this success, this research thesis aims to address some practical unknowns about field implementation of VisNIR spectroscopy and the prediction of *in situ* soil properties.

1.2. The challenge with *in situ* VisNIR spectroscopy

Aside from instrument development, the most significant challenges for employing VisNIR spectroscopy *in situ* are variability in soil moisture, temperature, and

structure (Bricklemeyer and Brown, 2010). These factors, henceforth referred to as *in situ* effects, affect the VisNIR spectra and are variable under *in situ* conditions. Water content has a strong non-linear effect on soil spectra. Under *in situ* conditions, soil moisture will vary, which can lead to poor accuracy when predicting soil properties with *in situ* VisNIR spectroscopy.

Soil properties are predicted from their VisNIR spectral reflectance by creating models that use existing data housed in “libraries” that contain both soil spectral data and soil property data. VisNIR libraries contain VisNIR spectra collected on dried ground soils. There are VisNIR spectral libraries that contain hundreds or thousands of regional, national, or international samples (Waiser et al., 2007; Brown et al., 2007; Wijewardane et al., 2020). Such libraries cannot be used to directly predict soil properties using *in situ* spectra due to the *in situ* effects on the spectral reflectance. To use dried ground spectral libraries to predict soil properties using *in situ* spectra, the library and the *in situ* spectral data need to be transformed to remove interferences from *in situ* effects. Another approach is to build new *in situ* soil spectral libraries, but a spectral transformation would be the most efficient method, as it bypasses the need for sample collection associated with new locations.

Calibration models using *in situ* spectral libraries have been successful and demonstrate the ability of VisNIR to predict soil properties with *in situ* effects. In 2001, Hummel et al. (YEAR) scanned Illinois soils at varying moisture contents to predict soil organic matter and moisture. Simulated *in situ* spectral data have been created by scanning moist, intact soil cores. Calibration models from these field-moist intact scans

successfully predicted soil clay, fine clay, organic C, and inorganic C (Waiser et al., 2007; Morgan et al., 2009). Using an on-the-go VisNIR probe, similar to the VisNIR penetrometer, Brickley and Brown (2010) found that although on-the-go VisNIR was not able to distinguish subtle C variances in soils, clay content could be predicted with hybrid modeling with a standard error of prediction (SEP) of 69.4 g kg⁻¹ as compared to a similar laboratory model with an SEP of 53.1 g kg⁻¹.

One notable and successful approach to combat the *in situ* effects on soil spectra is the implementation of a spectral transformation, such as external parameter orthogonalization (EPO) when using dried ground soil spectral libraries for soil characterization predictions. The EPO transformation was first developed by Roger et al. (2003) to remove the effects of temperature on fruit juice spectra. Next, Minasny et al. (2011) demonstrated the effectiveness of EPO using dried ground and rewet soils. Ge et al. (2014) successfully predicted soil properties using spectra from moist and intact soil samples and a dried-ground library by implementing the EPO to remove the soil moisture effect. They also concluded that the soil moisture content of the sample was not needed to predict clay and organic C content on moist and intact soil cores. Although the EPO was successful at transforming spectra to match existing dried ground spectral libraries, there improvement was greater for clay content predictions than organic C predictions.

Recently, Ackerson et al. (2017) demonstrated that the EPO transformation was effective for measuring clay content using a penetrometer-mounted VisNIR spectrometer on soils of varying parent materials. By using an EPO-partial least squares model

combination, *in situ* VisNIR spectroscopy predicted clay content with a root mean squared error (RMSE) ranging from 70 to 98 g kg⁻¹ and r² of 0.60 to 0.82. Angelopoulou et al. (2020) conducted a review of multivariate methods for SOC estimations and found that prediction capabilities of various models ranged from r² of 0.1 to 0.99 and RMSE of 0.04 to 13.1%.

Other researchers have used the approach of direct standardization (DS) to convert soil spectra collected from *in situ* soils to formats that can be predicted with a dried ground calibration model (Wang et al., 1991; Ji et al., 2015). This approach worked well in some cases because the range in soil water content was not very large (Ji et al., 2015). When the method was tested on intact soils with a wide range in particle size and moisture, the residuals of the model were found to be correlated to water content (Ackerson, 2016) indicating that DS has its limitations. It is likely that DS does not perform as robustly as EPO because DS is a linear transformation, while EPO is a multi-dimensional approach, removing the effects of “unwanted” parameters in orthogonal space (Roger et al., 2003; Ji et al., 2015).

1.3. Developing an *in situ* VisNIR device

Several groups have made progress towards making a VisNIR spectroscopy device capable of collecting truly *in situ* soil spectra. Mouazen et al. (2005) made one of the first strides towards an *in situ* instrument with the development of a fiber-type VisNIR spectrophotometer to measure soil moisture in the 306-1711 nm range. This system was implemented for the prediction of soil carbon and pH and later with

phosphorus in Mouazen et al. (2007). In 2010, Brickleyer and Brown tested one of the first commercially available VisNIR on-the-go sensors (Veris® Technologies Inc., Salina, KS, USA). Upon testing in Montana, Brickleyer and Brown (2010) found that soil heterogeneity and variation in moisture decreased the accuracy of soil property estimation as compared to laboratory testing. Rodionov et al. (2015) developed a VisNIR reflectance measuring chamber to be collected on a tractor. Soil organic carbon could be estimated with a standard error of 1.12 g kg⁻¹.

Poggio et al. (2015) developed a new VisNIR penetrometer fore optic capable of collecting soil VisNIR spectra *in situ*. Compared with an ASD contact probe (Malvern Panalytical Company, Longmont, CO, USA), this new fiber-optic cable yielded only a slight performance decrease. Brickleyer and Brown (2010), Rodionov et al. (2015), and Cho et al. (2017) performed similar testing and reported comparable findings. Ackerson et al. (2017) employed a penetrometer mounted with VisNIR (ASD spectrophotometer) to predict clay content in Texas. Further developments have incorporated a load cell, ultrasonic depth sensor, and a GPS receiver to create a multi-sensing system for the collection of true *in situ* vertical soil sensing (Wijewardane et al., 2020).

While a handful of research groups are testing VisNIR spectroscopy *in situ*, there is little information on data acquisition protocols. Namely, some programs have implemented a system where the VisNIR penetrometer is pushed into the ground multiple times within a square meter and spectra are averaged with depth to predict clay and organic C in that space. Other programs have relied on one or two sets of “pushes”

to provide spectral information. Whether spectral averaging improves property predictions has not been thoroughly explored. This is an important component to the development of this research if spectra are to be compared and prediction made across programs.

1.4. Spectral averaging and processing

Implementation of VisNIR spectroscopy from dried ground soil samples to characterize soils has been used in soil science for decades (Chang et al., 2001; Shepherd and Walsh, 2002; McCarty et al., 2002). In the laboratory, usually two scans of dried and homogenized soil are averaged. For *in situ* scanning, especially from a penetrometer, there are no defined protocols. Some researchers average spectra of the same soils (Ackerson et al., 2017; Wijewardane et al., 2020), and others make multiple soil property predictions from several spectra of the same sample (Wilke, 2010). Beyond averaging, preprocessing choices also have variances. Most average to 10 nm and filter using the Savitsky-Golay transformation with a second-order filter (Savitsky and Golay, 1964). Spectra can then be smoothed following methods such as Brown et al. (2006) or Waiser et al. (2007). After converting reflectance into absorbance, taking the first derivative is common (Ackerson et al., 2017). Derivatives are thought to be useful in picking up small differences in spectral curves and shapes at certain wavelengths where chemical overtones might show up, even if subtle. Overall, there is a lack of consensus among soil scientists using VisNIR as to what processing techniques are required for

representative spectra, even though standardization of methods among researchers may improve development of such proximal soil sensors (Viscarra Rossel et al., 2011).

1.5. Modeling

Several models have been used for calibration of VisNIR spectral models. Linear models (such as ordinary least squares, principal component regression and partial least squares and linear discriminant analysis), and non-linear machine learning techniques have all been applied. Common machine learning options include neural networks, random forest, and convolution networks (Morellos et al., 2016; Stevens et al., 2013, Viscarra Rossel and Behrens, 2010). Calibration datasets can be strengthened with bagging or boosting, but this leads to the risk of overfitting or overestimating prediction capabilities of the technology. Although several modeling methods have been assessed, partial least squares regression (PLSR) has been consistently successful and is generally considered the standard for comparing any new method being tested (Ackerson et al., 2017; Wijewardane et al., 2020; Pei et al., 2018).

1.6. Spectral Predictions of Soil Properties

Wijewardane et al. (2016b) found that a regional EPO paired with dried ground soil samples from a national soil spectral library can yield soil property predictions comparable to those of laboratory results, but noted that high moisture soils often had poorer predictions. A significant consideration when using the EPO is the unknown effect of “regionality” of soils used for sourcing EPO information beyond matching

properties of interest for validation. Ackerson et al. (2015) showed that the EPO libraries created for soils of Brazil and temperate soils of Texas, USA, were not interchangeable because the type of clay varied from Fe/Al oxides and 1:1 silicate clays that predominate in the Brazilian EPO to greater dominance of 2:1 silicate clay in Texas. In another investigation, Ackerson et al. (2014) did find that the EPO of Texas, USA, was interchangeable with an EPO of soils from New South Wales, Australia.

Testing of the effect of regionality on spectral predictions is limited in EPO libraries, but it has been conducted extensively in dried ground libraries. Stenberg et al. (2010) suggests that large libraries spanning over soils with a wide variation in properties drives prediction errors in validation data sets in addition to a lack of sample homogeneity. Viscarra Rossel et al. (2016) found, however, that a global soil spectral dataset provided comparable estimates of soil property predictions as other studies conducted at continental or global scales. They also reported that filtering and standardizing global spectra helped to remove the effects of inconsistencies from varied sample preparation, measurement protocols, and instrumentation.

2. ROBUSTNESS OF A VISNIR-MOUNTED PENETROMETER METHODOLOGY: LIBRARY SELECTION, EPO PROJECTION, AND FIELD PROTOCOLS

2.1. Introduction

Spatially explicit, quantitative soil information is becoming increasingly important, especially information that quantifies soil property variation at depth, or along the soil profile. This data is needed in order to implement precision agriculture, produce spatial and temporal modeling of water, carbon, nutrient, and contaminant fluxes in addition to building digital soil maps (Minasny and McBratney, 2016; Vereecken et al., 2016; Viscarra Rossel and Bouma, 2016). Current practices require soil cores to be extensively collected and tested in the laboratory for characteristics such as clay or soil organic carbon (SOC) (Hartemink and Minasny, 2014). While proximal sensing is generally less accurate, it is scalable to millions of acres and has the potential, when coupled with remote sensing and statistical sampling algorithms, to collect data at the necessary spatial density and depth at scale (Adamchuk et al., 2017).

VisNIR spectroscopy has had success in predicting various soil characteristics from spectral libraries. Most often, it is used to predict properties such as clay, SOC, and other related properties (e.g., total nitrogen and cation exchange capacity) from spectra collected on dried, ground, and sieved (< 2 mm) soil (i.e., referred to as dried ground from here on). Soil spectral libraries created from dried ground soil samples exist to model and predict these soil properties from newly collected samples and their corresponding spectra (Waiser et al., 2007; Brown et al., 2007; Wijewardane et al.,

2020). The USDA-NRCS Kellogg Lab spectral library is particularly useful because it is publicly accessible, large (~20,000 samples and growing) and covers many soils across the USA. These libraries often list the soil spectra at 10 nm increments from 500 to 2450 nm along with full or partial soil characterization. Most common soil characteristics in soil spectral libraries include sand, silt, clay, total C, carbonate, pH, and cation exchange capacity (Chang et al., 2001; Shepherd and Walsh 2002; McCarty et al., 2002).

While VisNIR spectroscopy has long been used in soil science for the prediction on dried ground soil samples, there has been growing interest in using VisNIR spectroscopy to predict soil properties from *in situ* spectra. Recent efforts have been made toward creating a penetrometer-mounted VisNIR spectroscopy system for the real-time prediction of soil properties (Ackerson et al., 2017; Wijewardane et al., 2020). Aside from instrument development, the most significant challenges for employing VisNIR spectroscopy *in situ* are variability in soil moisture, temperature, and soil structure (Bricklemyer and Brown, 2010). These factors, henceforth referred to as *in situ* effects, affect the VisNIR spectra and are variable under *in situ* conditions. Water content, in particular, has a strong non-linear effect on soil spectra, and varies with depth and over time, which can lead to poor accuracy when predicting soil properties with *in situ* VisNIR spectra.

One approach for modeling and predicting soil properties from *in situ* spectra is to generate new spectral libraries based on *in situ* spectra rather than dried ground spectra. This approach has been implemented (Morgan et al., 2009; Waiser et al., 2007; Bricklemyer and Brown, 2010), but requires expense and time for new and extensive

sample collection. Furthermore, errors can still be expected due to the effects of varying soil moisture (Waiser et al., 2007). Alternatively, a spectral transformation could be used to remove the *in situ* effects on the soil spectra of interest.

Calibration models using *in situ* spectra have been successful and demonstrate the ability of VisNIR to predict soil properties with *in situ* effects. In one study, Hummel et al. 2001 scanned Illinois soils at varying moisture contents to predict soil organic matter and moisture. Simulated *in situ* spectral data have been created by scanning moist, intact soil cores. Calibration models from these field-moist intact scans successfully predict soil clay, fine clay, SOC, and inorganic C (Waiser et al., 2007; Morgan et al., 2009). Using an on-the-go VisNIR probe, similar to the VisNIR penetrometer, Brickley and Brown (2010) found that although on-the-go VisNIR was not able to distinguish subtle C variances in soils, clay content could be predicted with hybrid modeling with a standard error of prediction (SEP) of 69.4 g kg⁻¹ as compared to a similar laboratory model with an SEP of 53.1 g kg⁻¹.

One notable and successful approach to combat the *in situ* effects on soil spectra is the implementation of a spectral transformation, such as external parameter orthogonalization (EPO) when using dried ground soil spectral libraries for soil characterization predictions. The EPO transformation was first developed by Roger et al. (2003) to remove the effects of temperature on fruit juice spectra. Next, Minasny et al. (2011) demonstrated the effectiveness of EPO using dried, ground, and rewet soils. Ge et al. (2014) successfully predicted soil properties using spectra from moist and intact soils and a dried ground soil VisNIR spectral library by implementing the EPO to remove the

soil moisture effect from their scans prior to evaluation with the library. They also concluded that the soil moisture content of the sample was not needed to predict clay and SOC content on moist and intact soil cores. Although the EPO was successful at transforming spectra to match existing dried ground spectral libraries, the improvement was greater for clay content predictions than SOC predictions. Ackerson et al. (2017) further demonstrated that the EPO transformation was effective for measuring clay content using a penetrometer-mounted VisNIR spectroradiometer on soils of varying parent materials. By using an EPO-partial least squares model combination, *in situ* VisNIR spectroscopy predicted clay content with a root mean squared error (RMSE) ranging from 70 to 98 g kg⁻¹ and r² of 0.60 to 0.82.

Wijewardane et al. (2016a) found that a regional EPO paired with dried ground soil samples from the NRCS-Kellogg soil spectral library can yield soil property predictions comparable to those of laboratory results, but noted that high moisture soils often had poorer predictions. A significant consideration when using the EPO is the unknown effect of “regionality” of soils used for sourcing EPO information beyond matching properties of interest for validation. Ackerson et al. (2015) showed that the EPO libraries created for soils of Brazil and Texas, USA, were not interchangeable because the type of clay varied from iron and aluminum oxides and 1:1 silicate clays that predominate in Brazil to 2:1 silicate clays in Texas. In another investigation, Ackerson et al. (YEAR) did find that the EPO of Texas, USA, was interchangeable with an EPO of soils from New South Wales, Australia (2014).

Testing of the effect of regionality on spectral predictions is limited in EPO libraries, but it has been conducted extensively in dried ground spectral libraries. Stenberg et al. (2010) suggests that large libraries spanning over soils with a wide variation in properties drives prediction errors in validation data sets in addition to a lack of sample homogeneity. Viscarra Rossel et al. (2016) found, however, that a global soil spectral dataset provided comparable estimates of soil property predictions as other studies conducted at continental or global scales. They also reported that filtering and standardizing global spectra helped remove the effects of inconsistencies from varied sample preparation, measurement protocols, and instrumentation. Similarly, there has been limited testing of the effects of the pairings between dried ground spectral libraries and EPO libraries.

Other researchers have used the approach of direct standardization (DS) to convert soil spectra collected from *in situ* soils to formats that can be predicted with a dried ground calibration model (Wang et al., 1991; Ji et al., 2015). This approach worked well in some cases because the range in soil water content was not very large (Ji et al., 2015). When the method was tested on intact soils with a wide range in particle size and moisture, the residuals of the model were correlated to water content (Ackerson, 2016) indicating that DS has its limitations. It is likely that DS does not perform as robustly as EPO because DS is a linear transformation, while EPO is a multi-dimensional approach that removes the effects of “unwanted” parameters in orthogonal space (Roger et al., 2003; Ji et al., 2015).

Another critical factor when using *in situ* VisNIR spectroscopy to predict soil properties is proper methodology for scan averaging. When implementing an instrument such as the VisNIR-mounted penetrometer in the field, there needs to be knowledge as to the benefit, or lack thereof, of taking multiple scans to average for soil property prediction. Thus, it is critical to determine the number of scans, or rather number of pushes, needed with the VisNIR penetrometer to get enough quality spectra for the accurate and precise prediction of soil clay and SOC. There is a current lack of literature regarding this methodology.

In this study, soil property prediction from *in situ* VisNIR spectra will be investigated as an alternative to dried ground VisNIR spectra. More specifically, we (1) compared the prediction capabilities of clay and SOC from three soil spectral libraries, (2) assessed the effects on prediction accuracy and precision when pairing spectral libraries with different EPOs for the prediction of *in situ* soil properties, and (3) analyzed the accuracy of VisNIR prediction capabilities from replicated *in situ* spectra. Within the scope of these objectives, the relative influence of size or locality of the soil spectral library versus the choice of EPO on prediction capabilities was evaluated. We hypothesize that if a spectral library is diverse in its range of clay and SOC contents, then it will be able to predict clay and SOC on *in situ* VisNIR soil spectra, regardless of regionality.

2.2. Materials and Methods

2.2.1. Spectral Data Sets

Three dried ground spectral libraries were chosen for model calibration: the Texas Soil Spectral Library (TSSL; Ge et al., 2014), National Resource Conservation Service library (NRCS-Brown; Brown et al., 2007), and the Kellogg Laboratory Spectral Library (NRCS-Kellogg; Kellogg Soil Survey Lab, Lincoln, NE) (Table 1). Each library varies in size, soil characteristics, and region of origin. The TSSL contains 2,094 dried ground VisNIR spectra representing soils across Texas, which were collected using an ASD AgriSpec spectroradiometer (ASD, a Malvern Panalytical Company, Longmont, CO, USA). Clay content was determined via pipette method (Gee and Or, 2002) and SOC by dry combustion (Nelson and Sommers, 1996) less inorganic carbon measured by the Chittick's method (Dreimanis, 1962). The NRCS-Brown library contains dried ground VisNIR spectra of 3,659 soils from across the continuous United States, which were collected with an ASD FieldSpec Pro spectroradiometer (ASD, a Malvern Panalytical Company, Longmont, CO, USA). Clay content was measured by pipette method. Soil organic carbon was measured using the modified Walkley-Black method (Walkley and Black, 1934) or by subtraction of inorganic carbon measured by Manometric HCL treatment (Soil Survey Staff, 1996) from total C by dry combustion (Nelson and Sommers, 1996). The NRCS-Kellogg library consists of over 60,000 dried ground soil spectra from across the globe, which were collected by an ASD LabSpec spectroradiometer. Clay and SOC were characterized similarly to the NRCS-Brown library.

Table 1. Summary of dried ground soil spectral libraries used in the study.

	TSSL (Texas Soil Spectral Library)	NRCS-Brown Library	NRCS-Kellogg Library
Number of samples	2,094	3,659	60,787
Geographic extent	Texas	United States	US + Other Countries
Spectroradiometer	ASD Agri Spec	ASD Field Spec Pro	ASD Lab Spec
Reference	Ge et al., 2014	Brown et al., 2007	Wijewardane et al., 2020

The NRCS-Kellogg library contains data from soils that are mineralogically dissimilar from our study area (e.g., Andisols and Oxisols). To improve model predictions with large geographically diverse libraries, it is often beneficial to calibrate models on a subset of data from complete libraries (Viscarra Rossel et al., 2016). We began sub-setting the NRCS Kellogg library by removing records with clay content greater than 900 g kg⁻¹ or SOC greater than 500 g kg⁻¹. Next, we compared spectra from our study region and removed spectra from the NRCS-Kellogg library that fell outside of the convex hull of 2 principle components (RStudio Team, 2020). The resulting NRCS-Kellogg data set was reduced from 60,087 to 20,034 spectra (Table 2).

Table 2. Summary statistics for the soil characterization data in each library used for calibration and the validation data. EPO is external parameter orthogonalization.

Dataset	n	Min.	Median	Max.	s
----- g kg ⁻¹ -----					
<i>Clay Content</i>					
TSSL	2,002	0	276	882	200
NRCS-Brown	3,658	1	224	900	168
NRCS-Kellogg	20,034	0	177	900	151
Illinois Validation		115	283	487	85
Texas EPO	161	27	277	681	158
Midwestern EPO	190	31	358	540	112
Nebraska EPO	85	320	440	540	69.0
<i>Soil Organic Carbon Content</i>					
TSSL	1,987	0	3.1	79.7	7.3
NRCS-Brown	3,309	0	4.3	226	17
NRCS-Kellogg	38,899	0	0	499	30
Illinois Validation	98	0	4.8	26.7	6.0
Texas EPO	NA	NA	NA	NA	NA
Midwestern EPO	190	1.7	11.7	53.2	8.2
Nebraska EPO	85	2.3	12.0	25.0	6.6

2.2.2. EPO Development

Three EPO projections were used for spectral transformation to remove *in situ* effects on spectral data. External parameter orthogonalization projection can correct *in situ* effects on field-collected spectra, which enables VisNIR spectra from dried ground soil spectral libraries to be used to calibrate VisNIR soil spectral models for the prediction of clay and SOC. These *in situ* effects, primarily soil water content and heterogeneity associated with soil intactness, have been successfully removed by EPO transformation (Ge et al., 2014; Ackerson et al., 2017; Wijewardane et al., 2020) and evaluated extensively (Roger et al., 2003; Minasny et al., 2011).

All EPO projections used pairs of VisNIR spectra from the same soils scanned dried ground and *in situ* using the VisNIR-mounted penetrometer. One EPO projection was developed using a set of scans from Texas soils with parent materials of weakly consolidated shale and sandstone, residuum, old and recent alluvium; one EPO was created using Midwestern soils weathered primarily from primarily loess and alluvium (Nebraska, Iowa, and South Dakota); and one EPO was created for Nebraska soils all from loess deposits. Summaries of SOC and clay content for the EPO datasets are in Table 2. The spectral data for each EPO dataset were from different ASD spectroradiometers, which were AgriSpec for the Texas EPO and LabSpec for the Midwestern and Nebraska EPOs. Each EPO was later calibrated with the optimal number of principle components that provided the lowest combination of RMSE and bias.

2.2.3. Field Collection of *in situ* Soil Spectra

The *in situ* VisNIR-mounted penetrometer data, used as a validation test set for all model calibrations (varying in library and EPO), were collected across three fields in Martinsville, IL, and three fields in Springfield, IL. All fields were conventionally tilled and row cropped. Sites within each field were chosen to maximize variability in soil properties by choosing among soil mapping units and topographic characteristics of the landscape. All soils measured in this field investigation are derived from loess and alluvium. The clay mineralogy of these soils is primarily mixed and smectitic, and the soils are predominantly Mollisols with a few Alfisols (Soil Survey Staff, 2004; Table 3).

Table 3. Taxonomy of soils that were scanned using the VisNIR-mounted penetrometer for the Illinois validation dataset. All soils were Mollisols or Alfisols.

Mapped Soil Series	Soil Taxonomy	n
Buckhart silt loam	Fine-silty, mixed, superactive, mesic Oxyaquic Argiudolls	9
Ipava silt loam	Fine, smectitic, mesic Aquic Argiudolls	29
Osco silt loam	Fine-silty, mixed, superactive, mesic Typic Argiudolls	13
Sable silty clay loam	Fine-silty, mixed, superactive, mesic Typic Endoaquolls	4
Bluford silt loam	Fine, smectitic, mesic Aeric Fragic Epiaqualfs	12
Blair silt loam	Fine-silty, mixed, superactive, mesic Aquic Hapludalfs	4
Atlas silt loam	Fine, smectitic, mesic Aeric Chromic Vertic Epiaqualfs	
Cisne silt loam	Fine, smectitic, mesic Mollic Albaqualfs	13
Newberry silt loam	Fine-silty, mixed, superactive, mesic Mollic Endoaqualfs	8
Ebbert silt loam	Fine-silty, mixed, superactive, mesic Argiaquic Argialbolls	12
Hoyleton silt loam	Fine, smectitic, mesic Aquollic Hapludalfs	5

n = number of samples

At each sampling location, four sets of profile scans were collected by pushing a VisNIR-mounted penetrometer into the ground in one-inch (2.5 cm) increments, as marked on the penetrometer shaft, with a hydraulic soil probe (Giddings Machine, Fort Collins, CO). VisNIR profiles scans at each sampling location were distributed roughly equally along an approximately 50-cm transect. Instrumentation of the VisNIR penetrometer used in this study is described in detail by Wijewardane et al. (2020).

In addition to scans collected with the VisNIR penetrometer, a representative soil core at each site was collected and sealed in a 6-cm diameter plastic sleeve and capped for transport to the laboratory. Soil cores were collected approximately 10-25 cm away from locations of VisNIR profile scans. Approximately five 5-cm sections along each core profile were subsampled for laboratory analysis. Sections were chosen to represent the variety of soil horizons and variability present in each profile. These

sections were air-dried and ground to pass a 2-mm sieve, and scanned again by the same ASD Field Spec Pro (ASD, a Malvern Panalytical Company, Longmont, CO, USA). An Illinois soil spectral dataset was used for the validation of models built with each of these three libraries. Clay content was measured by pipette method (Gee and Or, 2002) and SOC was measured by dry combustion (Nelson and Sommers, 1996) less inorganic C measured by modified pressure calcimeter (Sherrod et al., 2002).

2.2.4. Spectral Processing

Prior to model building and analysis, all spectra (i.e., dried ground and *in situ*) were filtered using the Savitsky-Golay transformation with a second order filter and 11-nm window size (Savitzky and Golay, 1964). Spectra were cut to include wavelengths in the 500 to 2450 nm range and averaged to 10 nm intervals to decrease data size and processing times. All filtered reflectance spectra were transformed to absorbance via log (1/reflectance).

Once processed by the methods listed above, *in situ* spectra of the Illinois validation dataset were grouped by farm, field, location within the field, and depth. The *in situ* spectra were matched by sampling depth to the soil sampled for laboratory analysis and dried ground VisNIR scanning. The *in situ* spectra that were taken within the depth range of the selected soils were kept and referred to as matched *in situ* spectra. One challenge with *in situ* VisNIR acquisition is that due to arrangement of sampling locations, samples for replicated scans and laboratory analysis are not collected in identical locations (Fig. 1). Subsequently, due to variability in soil horizon depths,

VisNIR spectra collected from replicate profile scans at the same depths may not represent the same soil horizon (Fig. 2a). To ensure spectra originated from the same horizon/material, matched *in situ* spectra were then visually assessed for quality. This quality assessment primarily required visually identifying any spectra that contained any spectral forms with a different overall shape compared to others in the set from replicate scans (Fig. 2b).

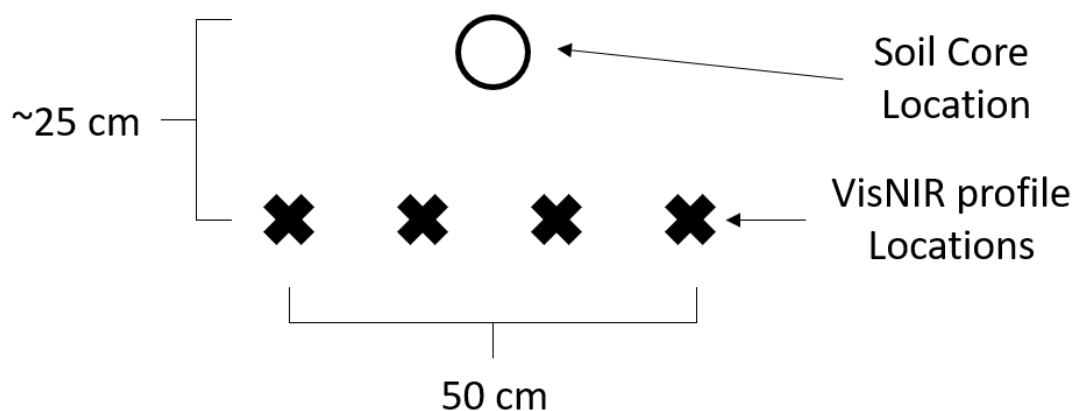


Figure 1. Plainview of sample collection layout. X's and O's represent the locations of VisNIR spectra profile and soil sample locations, respectively.

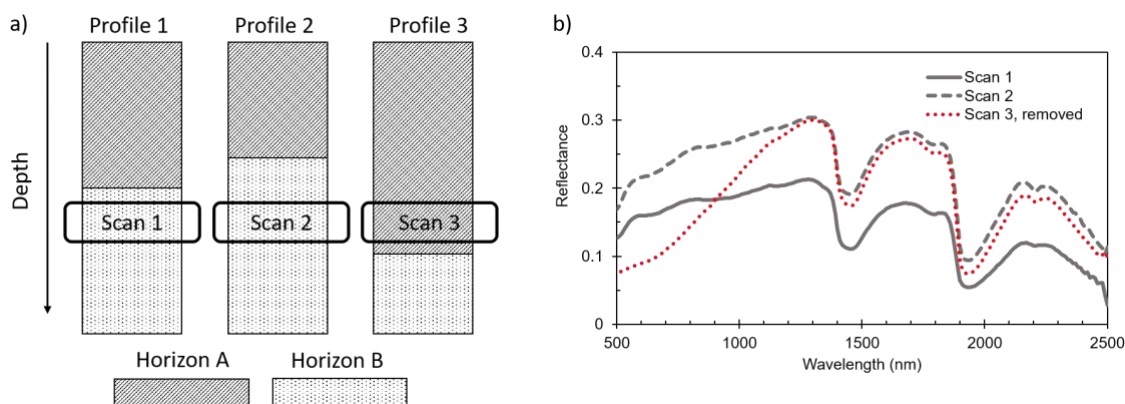


Figure 2. Three *in situ* VisNIR spectra collected at the same location and depth. Spectra highlight variability that can be observed.

Matched sets of spectra containing between one and four *in situ* spectra were averaged, depending on the quality and the spectra that passed visual inspection. Libraries and EPO projections were paired for developing model predictions, and predictions were compared to laboratory measurements. The r^2 , RMSE, and bias values were calculated and compared to evaluate model performance.

2.2.5. Model Development and Analysis

Two types of prediction models were created so the model performance could be assessed: dried ground and *in situ* prediction models. First, the suitability of each of the three libraries (i.e., TSSL, NRCS-Brown, and NRCS-Kellogg) to predict clay and SOC from the Illinois samples was evaluated by comparing dried ground VisNIR spectral interpretations with laboratory analysis. This provided an evaluation of the Illinois soils independent of *in situ* conditions. Second, the *in situ* VisNIR spectra from the Illinois

soils were evaluated using the same dried ground libraries (i.e., TSSL, NRCS-Brown, and NRCS-Kellogg) with EPO projections from the EPO datasets (i.e., Texas EPO, Midwestern EPO, Nebraska EPO) to predict clay and SOC. This provided an assessment of the Illinois soils under *in situ* conditions using the EPO-transformed libraries.

Partial least squares models (PLS) were used to predict clay and SOC from the spectral libraries for all spectra. These models were calibrated using the statistical software R and PLS package (R Core Team, 2015). All models were calibrated with the respective dried ground libraries, independent of the Illinois validation data. Each spectral library was used to first calibrate separate PLS models for the prediction of clay and SOC on the dried ground spectral data.

Next, an EPO projection was implemented. The EPO matrix was constructed from *in situ* and dried ground VisNIR spectra following the methods of Minasny et al. (2011). EPO projections were used to transform both the *in situ* validation spectra as well as the dried ground library used to calibrate the prediction model. Each EPO dataset was used to create a unique EPO projection and to transform each dried ground library and *in situ* Illinois spectra. After EPO transformations, the transformed spectral library was used to create a prediction model for clay and SOC. Predictions for the *in situ* Illinois spectra are made and evaluated compared to laboratory data.

All models were calibrated with optimal number of PLS natural latent variables (NLV) and EPO principle components (PC) for the Illinois validation dataset. The NLV values were tested and selected based on a 30% holdout sample of the Illinois validation dataset. For *in situ* predictions, each pairing of library and EPO were calibrated using the

optimum pairing of NLV and PC for the validation dataset. The predicted datasets were each compared to their corresponding wet chemistry values. Each model was assessed using RMSE, bias, and r^2 (Willmott, 1981). For the purposes of this paper, RMSE was used to evaluate the accuracy of the EPO-PLS models, bias was used to assess over or under-prediction tendencies, and r^2 was used to represent the precision of these models.

Once optimum library and EPO projections were selected, the usefulness of multiple scans (i.e., pushes of the VisNIR penetrometer) on precision, bias, and accuracy was evaluated. At each site, four scans were made with the VisNIR-mounted penetrometer; however, matching of penetrometer scans with depth and visual cleaning for spectra with irregular shape removed some of the replicate scans. Upon completion of model development and analysis, soils that had four *in situ* spectra used for prediction were used to assess the usefulness of multiple scans. First, all four scans were used for prediction of clay and SOC contents, matching the exact predictions of data presented prior. Then, a random spectra of each soil was removed to assess the prediction accuracy when three spectra for the soil were used for prediction. This was repeated twice more to assess the prediction capabilities with two and one spectra. Due to robustness of predictions, the TSSL library and Texas EPO were used. Model performance metrics were used to assess benefit to having multiple scans with the VisNIR-mounted penetrometer to predict clay and SOC.

2.3. Results

2.3.1. Dried Ground Library Performance

Clay content prediction performance for Illinois dried ground soil samples was similar for all three libraries evaluated. The RMSE of clay content predictions for all three soil spectral libraries were between ± 39 to 50 g kg^{-1} , and all biases were less than an absolute value of 10 g kg^{-1} (Fig. 3; Table 4). The NRCS-Kellogg library had the lowest RMSE of 39 g kg^{-1} ; however, the NRCS-Kellogg library had the largest absolute bias of 9 g kg^{-1} . The TSSL and NRCS-Brown models had slightly larger RMSE than the NRCS-Kellogg but had negligible bias. All the models evaluated performed well for clay content predictions regardless of library. For SOC, all three libraries had similar performance with RMSE values of 3.7 to 3.9 g kg^{-1} ; however, the bias in the Kellogg library was the highest at 1.1 g kg^{-1} (Fig. 4; Table 4). For brevity, only the TSSL and NRCS-Kellogg libraries prediction graphs are displayed.

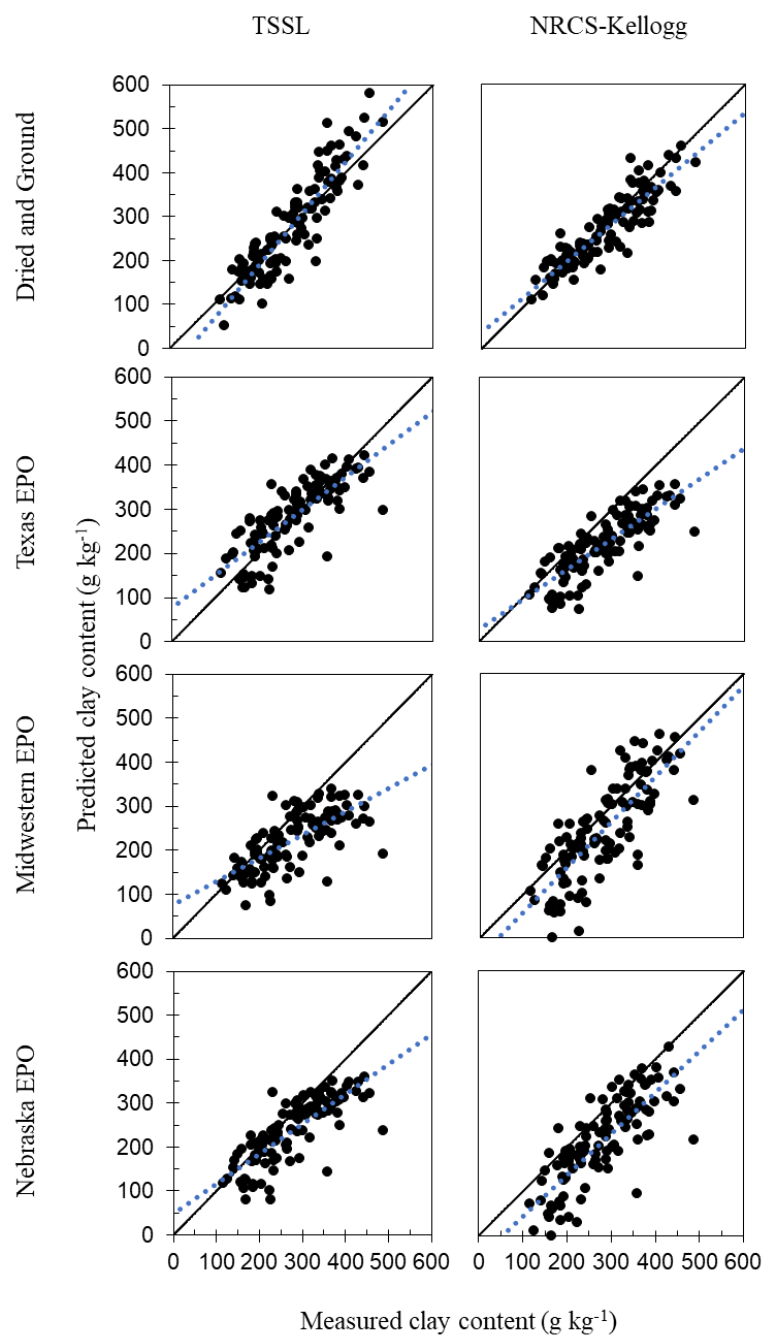


Figure 3. Relationships between measured and predicted clay content in dried ground and *in situ* soil using the TSSL and NRCS-Kellogg libraries with Nebraska, Midwestern, and Texas EPO datasets.

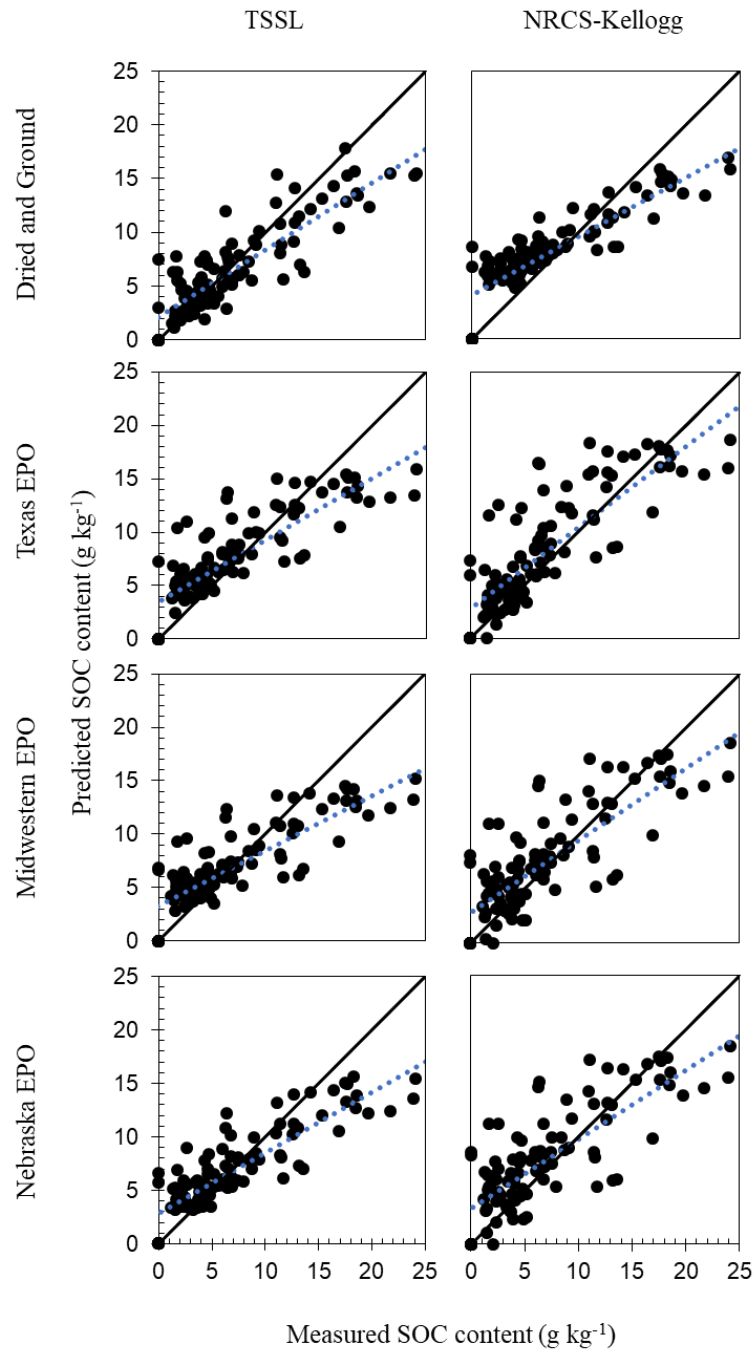


Figure 4. Relationships between measured and predicted SOC in dried ground and *in situ* soil using the TSSL and NRCS-Kellogg libraries with Nebraska, Midwestern, and Texas EPO datasets.

2.3.2. *In situ* Predictions with EPO projections

Overall, predicting clay and SOC with *in situ* spectral measurements reduced precision (r^2), but model performance on accuracy and bias varied with dried ground library selection. For the prediction of clay content on *in situ* soil spectra of the validation dataset, r^2 ranged from 0.63 (NRCS-Brown library with Midwestern state EPO projection) to 0.70 (NRCS-Brown library with Nebraska EPO projection). The Texas EPO projection and TSSL model yielded the best prediction performance regarding accuracy and bias (RMSE of 51 g kg⁻¹ and bias of 4 g kg⁻¹). Interestingly, the Texas EPO projection used with both the TSSL and NRCS-Brown models yielded an RMSE of 51 g kg⁻¹ clay, yet bias varied greatly (4 g kg⁻¹ with the TSSL model and -16 g kg⁻¹ clay with the NRCS-Brown model). Although the NRCS-Kellogg model had the best performance on dried ground soils, the NRCS-Kellogg library had poor prediction performance with all three EPO projections (Fig. 3; Table 4).

For the prediction of SOC from *in situ* spectra, the TSSL was the most consistent predictor of SOC with all three EPO projections with RMSE ranging from 3.5 to 3.8 g kg⁻¹ and bias ranging from -0.1 to 0.6 g kg⁻¹ SOC. The NRCS-Brown library models predicted SOC from *in situ* spectra with an RMSE over 5 g kg⁻¹ with all EPO projections, and biases ranging from 3 to 9 g kg⁻¹. Even though *in situ* spectra were not as good at predicting clay content as dried ground spectra, *in situ* spectra coupled with the NRCS-Kellogg library were able to predict SOC on the validation soils with an RMSE comparable to its dried ground predictions. The RMSE values of the *in situ* models built with the NRCS-Kellogg library with all three EPO projections ranged from

4.0 to 4.7 g kg⁻¹ and bias ranged from 1.9 to 3.2 g kg⁻¹ SOC (Fig. 4; Table 4). Overall, bias disparities become more significant in EPO prediction models as compared to dried ground model predictions. This bias could be a reflection of differences in laboratory method for prediction of SOC.

Table 4. Description of prediction outcomes for clay and soil organic C using the three dried ground spectral libraries along with external parameter orthogonalization (EPO) projections for prediction of *in situ* soil spectra collected with the VisNIR-mounted penetrometer.

	TSSL			NRCS-Brown			NRCS- Kellogg		
	r ²	RMSE	Bias	r ²	RMSE	Bias	r ²	RMSE	Bias
	----- g kg ⁻¹ -----			----- g kg ⁻¹ -----			----- g kg ⁻¹ -----		
	<i>Clay Content</i>								
Dried and Ground	0.81	50	1	0.69	47	2	0.80	39	-9
Texas EPO	0.64	51	4	0.69	51	-16	0.67	77	-61
Midwestern EPO	0.49	83	-56	0.63	72	-42	0.63	75	-38
Nebraska EPO	0.64	65	-41	0.70	64	-41	0.62	93	-69
	<i>Organic Carbon Content</i>								
Dried and Ground	0.61	3.8	0.4	0.80	3.9	0.6	0.81	3.7	1.1
Texas EPO	0.66	3.8	0.6	0.62	5	3	0.68	4.7	3.2
Midwestern EPO	0.66	3.8	-0.1	0.68	7.9	6	0.70	4.0	1.9
Nebraska EPO	0.73	3.5	-0.2	0.69	9.4	9	0.70	4.1	2.3

2.3.3. PLS and EPO Model Parameterization

The number of NLVs for PLS models provided insight to the model complexity required for an optimum prediction. The NRCS-Kellogg and NRCS-Brown libraries

required eight and two NLVs for the predictions of clay and SOC on dried ground soils, respectively. The TSSL required only five NLV for clay, but seven for SOC (Table 5). Most of the models that paired the dried ground library with an EPO required one or two NLVs and PCs. Exceptions included the combination of the Midwestern and Nebraska EPOs with the NRCS-Kellogg library for clay content models and with TSSL or NRCS-Brown library for SOC models (Table 5).

Table 5. Number of principle components (PC) and/or natural latent variables (NLV) used in clay and soil organic carbon models. Principle components and latent variables were optimized for best performance outcomes (RMSE and r^2) for each external parameter orthogonalization (EPO) model.

	TSSL		NRCS-Brown		NRCS-Kellogg	
	NLV	PC	NLV	PC	NLV	PC
	<u>Counts</u>					
	<i>Clay Content</i>					
Dried and Ground	5	-	8	-	8	-
Texas EPO	2	2	2	2	2	2
Midwestern EPO	2	2	2	2	5	1
Nebraska EPO	2	2	2	2	8	2
	<i>Soil Organic Carbon Content</i>					
Dried and Ground	7	-	2	-	2	-
Texas EPO	2	2	2	1	1	2
Midwestern EPO	2	2	6	2	1	2
Nebraska EPO	5	2	1	2	1	2

For most library-EPO combinations, EPO-PLS models required fewer NLV's than corresponding dried ground models. This behavior is common in EPO-PLS applications (Ackerson et al., 2017). It is important to note, however, that this behavior

is not universal and that some library-EPO combinations required more NLVs, highlighting the need for model-specific calibrations.

2.3.4. Replicate spectra influence on prediction performance

Few scans were removed with visual inspection for varying shape and spectral features (Fig. 5). The number of total spectra used for each soil characterization, however, did not impact model performance for clay or SOC content predictions. For clay content, r^2 varied from 0.66 to 0.74 with no clear pattern with increasing scans. The RMSE values followed a similar pattern, ranging from 47 to 54 g kg⁻¹ with no clear trend or preference for higher or lower number of scans. The bias, however, was lower for the three and four replicate scan groups (-9 g kg⁻¹) as compared to -11 g kg⁻¹ of the one and two scan groups. For SOC predictions, r^2 decreases slightly with an increase in the number of scans used for prediction from 0.75 to 0.72. The RMSE values are consistent for all numbers of scans ranging from 2.8 to 2.9 g kg⁻¹. Bias varies slightly with no consistent pattern and ranges from 1.3 to 1.5 g kg⁻¹ (Table 6).

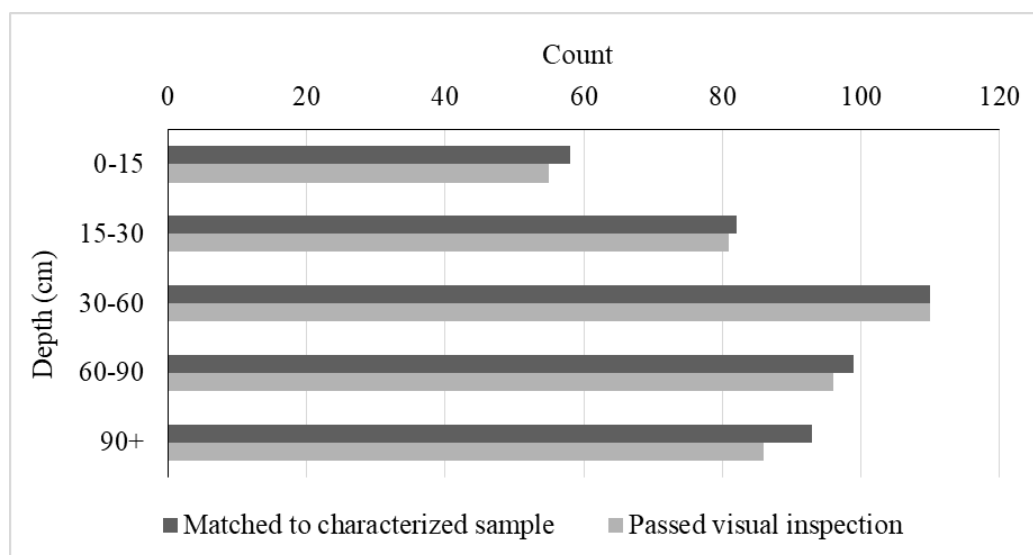


Figure 5. Counts of spectra pre- and post-visual inspection. Visual inspection removed spectra of dissimilar shapes and features from others collected at the same location and depth.

Table 6. Description of prediction outcomes for clay and soil organic C using the TSSL and Texas external parameter orthogonalization (EPO) for predictions made with one to four scans (i.e., pushes) or replicates of spectra.

# of Scans	Clay			Organic Carbon		
	r^2	RMSE	Bias	r^2	RMSE	Bias
	----- g kg ⁻¹ -----			----- g kg ⁻¹ -----		
1	0.72	50	-11	0.76	2.8	1.5
2	0.74	47	-11	0.75	2.8	1.3
3	0.66	54	-9	0.73	2.9	1.3
4	0.68	53	-9	0.72	2.9	1.4

2.4. Discussion

2.4.1. Model Performance

Although slight variations exist among the predictions, all soil spectral libraries seem to be viable options to predict clay and SOC with dried ground soils. Although

TSSL contains only Texas soils, it was able to accurately and precisely predict both clay and SOC contents on soils from Illinois. These results suggest that for the soils used in this study, library selection has little effect on dried ground model performance.

The Texas EPO projection paired with the TSSL model yielded some of the most accurate and precise predictions of both clay and SOC contents. The Texas EPO paired with the TSSL had the lowest RMSE and absolute bias of all *in situ* clay content predictions. The Texas EPO paired with the TSSL had the second lowest RMSE and had absolute bias within 0.2-0.4 g kg⁻¹ of the best performing *in situ* SOC models. Additionally, models paired with the Texas EPO projection generally needed the least number of PCs and NLVs, indicating both that the models are not being overfit to the dataset and the robustness of the EPO projection.

The soils represented by Texas data (TSSL and Texas EPO) are the most dissimilar to Illinois soils. Soils in the Illinois dataset were predominantly udic and aquic Alfisols and Mollisols, while soils from the Texas data set included udic, ustic, and aridic moisture regimes and represented Alfisols, Mollisols, Vertisols, Inceptisols, and Entisols. Despite the differences in soil composition, Texas data performed well for calibrating EPO-PLS models. This result suggests that, soil dissimilarity does not have a major impact on EPO-PLS interoperability for the soils in this study. However, previous work has found that soil dissimilarity can impact EPO-PLS model performance. Ackerson et al. (2015) found that EPO projections calibrated with Texas soils were not compatible with spectra collected on Brazilian soils and concluded that this lack of interoperability was due to extreme dissimilarity in soil composition. Given the results

of this study, it appears that there is a tolerable range in soil dissimilarity where EPO projections will be interoperable; provided the soils in question are not outside that range, EPO-projections should be transferable. Further investigations are needed to quantify this range and provide concrete guidance on the allowable dissimilarity ranges for EPO interoperability.

The strong performance of the Texas data could be attributed to several other factors. First, the TSSL and Texas-EPO, and Illinois validation spectra were collected by the same laboratory group using the same spectroradiometer. It may be more important to choose and soil spectral library collected with the same or similar spectroradiometer or perform a spectroradiometer calibration for the improvement of soil property predictions on *in situ* soils. These results suggest that EPO-PLS models can be interoperable despite being generated with pedogenically dissimilar soils in regard to parent material and mineralogy. Factors such as equipment choice and operator bias may have greater impact on interoperability than characteristics of soil in the underlying datasets. Further study is needed to determine to which factors control EPO-interoperability and how to best minimize the negative effects of these factors.

2.4.2. Replicate Scans

There is no clear advantage for using multiple VisNIR penetrometer scans for clay or SOC predictions. Although prediction accuracy is not necessarily improved, having multiple scans may increase confidence in knowing the scan was accurate for the soil of interest. Considering SOC predictions from *in situ* samples are generally less

accurate with VisNIR spectral models as compared to other spectral ranges (Yang et al., 2012), this may especially be a consideration for SOC measurements. VisNIR spectra reflect slight shadows and overtones of bond vibrations associated with SOC in soil, while in MIR these features are more prominent (Chen et al., 2016). For clay content predictions, additional spectral detail may not be as necessary for prediction depending on the accuracy desired, as there was a decrease in bias with increased number of replicate scans.

The VisNIR penetrometer has shown to be a viable option to measure soil characteristics, such as clay and SOC content *in situ*, with minimal soil removal or disturbance. Model calibration using a dried ground spectral library is possible and successful when a robust EPO projection is used with *in situ* spectra. More specifically, a spectral library collected with the same spectroradiometer as the validation dataset will likely yield the best prediction parameters and perhaps decrease bias and produce more accurate predictions. Alternatively, a spectral calibration could be used. When collecting data in the field, it may be advantageous to consider the accuracy and precision of interest to determine the number of scans (i.e., times to push the VisNIR penetrometer in the ground) of the same soil for the prediction of specific soil properties. Similarly, there was no conclusive evidence that lab methodology for SOC measurement impacted SOC predictions. There was variation in SOC prediction capabilities between the NRCS-Brown and NCS-Kellogg library models, even though SOC was measured by the same methods (modified Walkely-Black or dry combustion less inorganic carbon measured by Manometric HCL treatment), yet the TSSL models, containing SOC measured by dry

combustion less Chittick's inorganic carbon generally produced more accurate SOC predictions than both the NRCS-Brown and NRCS-Kellogg library models.

2.5. Conclusion

In regard to uniformity in methodology, there was no conclusive evidence suggesting that the method of SOC measurement in the laboratory impacted model performance. Results suggested that using different models of spectroradiometers impacted predictions of clay and SOC. When predicting soil characteristics on dried ground soil spectra, the choice of library impacts the prediction performance of SOC more than clay content. All libraries performed well and were capable of predicting both soil properties; soil spectral libraries were interoperable for dried ground spectra. When predicting soil characteristics on *in situ* spectra, the choice of dried ground library seemed to be more impactful than the choice of EPO projection dataset. The Texas EPO dataset was the most robust and was generally successful for all libraries. Visual removal of spectral outliers from replicate scans at the same depth removed few spectra, although perhaps an automation of spectral inspection may improve efficiency in future spectral analyses. Having more spectral replicates did not significantly improve prediction of clay or SOC, but may be helpful to identify outliers in spectral data. Further research may compare the ability of broad libraries and localized libraries to predict soil properties on the whole-farm level, or perhaps across a county to test how similar a predicted dataset must be for accurate model calibration. Furthermore, continued investigation of *in situ* soil property prediction with VisNIR is needed with data

collected by the VisNIR-Penetrometer to test the instrumentation and its ability to make real-time soil property predictions.

3. VISNIR SPECTROSCOPY FOR FIELD CLASSIFICATION OF SOIL PROFILES

3.1. Introduction

Reliable remote and proximal soil sensors can improve resolution of soil mapping and measure soil property changes from t management across landscapes (Adamchuk et al., 2004; Wenjun et al., 2019). Profile estimates of clay, organic carbon, calcite, and gypsum can be used to infer parent materials, texture, horizonation, and other soil characteristics that drive soil classification, landscape hydrology, affect nutrient cycling, and influence management decisions for agriculture and ecosystem services. Proximal and remote soil sensors are often relied upon for this information because of their low cost (relative to traditional chemical analyses), widespread availability, and most importantly, their ability to quantify soil properties across large spatial extents and at high spatial resolution (Adamchuk et al., 2004; Viscarra Rossel et al., 2011; and Demattê et al., 2015).

The visible and near infrared reflectance (VisNIR)-mounted penetrometer is one such proximal sensing technology that is particularly unique because it is being developed for soil profile characterization (Ackerson et al., 2017; Wijewardane et al., 2020). VisNIR spectroscopy has been used to rapidly and non-destructively characterize soil in the laboratory (Ben-Dor and Banin, 1995; O'Rourke and Holden, 2011). A significant benefit to using VisNIR spectroscopy is that multiple soil properties can be predicted from one measurement of soil spectral reflectance (Brown et al., 2006; Viscarra Rossel et al., 2006; Soriano-Disla et al., 2014; and Poggio et al., 2015). Soil

clay content, as well as organic and inorganic carbon content, are a few of the most common soil properties measured using VisNIR spectroscopy (Shepherd and Walsh, 2002; McCarty et al., 2002; Chang et al., 2011). While the prediction of soil properties, such as clay and carbon content, is faster and less destructive with VisNIR spectroscopy compared to traditional laboratory methods, laboratory spectroscopy still requires a great deal of sample preparation, including soil collection, transport, drying, grinding, and sieving. These transport and preparation processes limit the speed and cost efficiency of laboratory spectroscopy. While traditional laboratory analyses also require preparation time, the advantage of using them is that they are more precise than spectral predictions. There is a tradeoff between precision and cost when comparing laboratory spectroscopy and traditional laboratory measurements. Therefore, moving VisNIR spectroscopy to *in situ* field collection of spectra has the distinct advantage of removing the time and cost of transporting and preparing soil samples, thereby altering the weights between the balance between precision and cost.

A VisNIR spectrometer mounted on a penetrometer enables soil samples to be collected *in situ* and along the soil profile without pulling a soil core. The most significant challenge in employing VisNIR spectroscopy *in situ* is accounting for the effects of soil moisture, ambient temperatures, and soil structure on the soil spectra. These effects cause the VisNIR spectra collected on intact soils to be much different than those collected on the same soil dried, ground, and sieved to 2-mm (dried ground) soils in the laboratory (Bricklemyer and Brown, 2010). Ackerson et al. (2017) and Wijewardane et al. (2020) have shown that VisNIR spectra can be successfully collected

using a VisNIR-mounted penetrometer, and that the spectra can be converted to soil property data using dried ground spectral libraries with an external parameter orthogonalization (EPO) conversion of the spectra.

While the instrumentation is continuing to be developed, there is no published assessment of best methods for in-field data collection and processing. At the forefront of the discussion regarding collection and processing is the use of the EPO method to account for the intact nature of VisNIR soil spectra (variable moisture and heterogeneity) while leveraging soil spectral libraries at national and regional scales (Brown et al., 2006; Morgan et al., 2009; Wijewardane et al., 2016a; Ackerson et al., 2017). The two predominant options are to (1) use a transformation to remove the moisture and intact effects on the *in situ* spectra and predict soil properties from pre-existing dried ground soil spectral libraries or (2) build new *in situ* spectral libraries that represent the field moisture conditions of a survey. Both EPO and direct standardization are two such transformations that have been implemented to remove the effect of moisture from moist soil spectra to predict soil properties from pre-existing dried ground soil spectral libraries (Ge et al., 2014; Ji et al., 2015; Ackerson et al., 2017; Liu et al., 2020). Alternatively, *in situ* libraries have been developed with varying success and site specificities (Waiser et al 2007; Morgan et al., 2009; Minasny et al., 2011; Ge et al., 2014; Ackerson et al., 2017); however, variable moisture has been found to decrease prediction capabilities (Waiser et al., 2007; Morgan et al., 2009; Roudier et al., 2015).

Ultimately, the goal of using a VisNIR-mounted penetrometer is to survey soils across a landscape and to quantify characteristics of soil profiles. To accomplish the

field collection of data using this equipment, there are a few options regarding how to handle the soil profile data. These options all revolve around collecting multiple scans and averaging spectra. The hypothesis behind averaging multiple scans is that prediction accuracy can be improved. On the other hand, collecting more data also takes time. Bricklemeyer and Brown (2010) showed that homogenizing soils in the laboratory prior to scanning can increase the uniformity of the soil spectra, and therefore improve predictive capabilities (Bricklemeyer and Brown 2010). However, when the soil is scanned *in situ*, we do not know whether there is any benefit of collecting and averaging two sets of spectral data side-by-side. In the field, this could be akin to taking multiple pushes of the penetrometer into the soil. Another possible technique that could improve predictions is averaging spectra by horizon.

Because VisNIR can be used to predict clay content and other soil properties, we also wanted to test the utility of profile scans to classify soils into a specific soil series due to the cost and efforts required to classify soils by hand in the field. Several studies have investigated assignment of soils into classes or great groups based on principle component analysis (PCA) by spectra and texture, but few have considered soil series classification from a soil property prediction, such as clay content, alone. Similarly, there is need for proximal sensing to refine soil mapping units for land management. In the United States, soil maps are often limited to a scale of 1:24,000; hence, management activities requiring finer resolution field scales may not be as precise or accurate without finer resolution maps. Some soils are mapped as a complex of two series and our best

estimates of soil maps cannot always confidently distinguish between predicted soil series.

Having fine vertical- and spatial resolution clay content or soil texture data (the distribution of sand, silt and clay) allows land managers to estimate other soil properties, such as pore space, water holding capacity, depth to clay pans, or compaction potential. Currently, in the United States maps of soil series are often used to infer management limitations. For example, in Texas, there are landscapes mapped with three soil series (Burluson, Davilla, and Wilson), two of which are nearly impossible to differentiate in the field without collecting soil samples and performing proper taxonomic classification with supplementary laboratory data (e.g. particle size distribution). Because these soils are difficult to distinguish in the field, and are often mapped as a complex, there is need of proximal or remote measurements to help characterize and distinguish soils as it is seldom realistic to retrieve soil cores and thoroughly classify soils across a landscape. Soil property predictions with depth such as clay content from technology such as VisNIR could potentially help to classify soils. Although many axillary soil characteristics (e.g. clay films) are not detectable by VisNIR spectroscopy, predictions of clay content could help indicate applicable soil properties (filtration, structure, texture) without the inputs of holistic field classifications and can be more cheaply predicted by VisNIR than traditional field or laboratory classification.

The overall goal of this study was to investigate the potential of using a VisNIR-mounted penetrometer to both characterize soils from spectral predictions of clay content. More specifically, we focused on the prediction of soil clay content along the

soil profile and applied our best predictions to differentiating soil series that are difficult to differentiate in the field. First, two modeling approaches were considered to convert field moist intact spectra to estimate soil clay content. The approaches include using two different calibration techniques (1) an intact, field moist calibration and (2) a dried ground soil spectral library transformed using EPO. Second, the prediction accuracies were evaluated using individual soil spectra, averaging spectra from by side-by-side scans, averaging spectra by horizon, and averaging predictions rather than spectra. Finally, differences in prediction accuracy between surface horizons (A horizons) and subsurface horizons (E, B, C). were considered in order to evaluate the potential to apply predictions to a difficult soil classification example. Answering these objectives gives guidance to understanding the 1) context of using EPO transformations, 2) methodology for VisNIR-mounted penetrometer field campaigns, and 3) practical applications of *in situ* soil profile spectroscopy.

3.2. Materials and Methods

3.2.1. Calibration Datasets and Modeling

Two scenarios were used for creating the calibration model to convert field moist, intact spectral measurements into clay content. Data used for each scenario came from different sources. Scenario 1 used VisNIR scans collected intact and at field-moist conditions with associated laboratory measurements of clay content. The dataset is described in detail in Waiser et al. (2007). Scenario 2 used dried ground VisNIR spectra library described in Brown et al. (2006) with an EPO transformation matrix created

using paired intact, field moist and dried ground scans from the Waiser et al. (2007) dataset.

The Waiser et al. (2007) dataset (here on, named Waiser) used in Scenario 1 and Scenario 2 contains 270 pairs of scans and lab measurements from 32 soil cores collected from Erath and Comanche counties of Texas, USA (Table 7). The National Resource Conservation Service soil spectral library collected by Brown et al. (2006) (here on called NRCS-Brown library) contains 3,659 pairs of VisNIR spectra and lab data from the continuous United States. For all datasets, clay content was measured by pipette method (Gee and Or, 2002). Both data sets represent a wide range in clay content. While the Waiser data was limited geographically to central Texas, the NRCS-Brown library contains soils from the continuous United States.

Table 7. Summary statistics for soils and acquisition of VisNIR libraries

Dataset		Validation	Waiser	NRCS-Brown
Reference		Wilke, 2010	Waiser et al., 2007	Brown et al., 2006
Geographic Location		Milam & Lee Counties, Texas, USA	Comanche & Erath Counties, Texas, USA	Continuous United States
Spectroradiometer		ASD AgriSpec	ASD Field Spec Pro	ASD Field Spec Pro
Clay Content, g kg⁻¹	n	151	270	3,075
	Min	67	120	10
	Max	470	578	912
	Average	291	260	284
	s	100	130	177
	Median	307	260	262

The validation dataset was also collected in central Texas but from different counties (Table 7). The validation data set is described in detail in Wilke (2010). In general, the parent material (clayey Pleistocene alluvial terraces) in the validation dataset are represented in the Waiser data, and the Waiser data has a broader parent material representation (sandstone, shale, and limestone residuum, Pleistocene alluvial terraces, and floodplains). According to the county soil surveys, the soils in the validation set represent Burleson, Davilla, and Wilson soil series (Soil Survey Staff, n.d.). Burleson is a fine, smectitic, thermic Udic Haplustert on Pleistocene age terraces derived from clayey alluvium. Burleson soils have a clay loam surface and a clay subsurface texture. Davilla is a fine-loamy, siliceous, superactive, thermic Udic Haplustalf on Pleistocene age terraces derived from loamy alluvium. Davilla soils have a fine-loamy particle size class (for the first 50 cm of the argillic horizon, less than 35 g kg⁻¹ clay on a weighted average). Wilson is a fine, smectitic, thermic Oxyaquic Vertic Haplustalf on terraces or uplands from clayey alluvium of Quaternary age. Wilson soils have a fine particle size class (for the first 50 cm of the argillic horizon, there is greater than 35 g kg⁻¹ weighted average clay).

Although there are distinct differences noted in the taxonomy between Davilla and Wilson soil series, these soils are nearly impossible to distinguish in the field. Due to resolution limitations of soil maps, there is uncertainty as to where soil series boundaries lie. Additionally, their soil characteristics may be so similar (sometimes within 50 g kg⁻¹ clay content) that even laboratory data may not always distinguish (Figure 6).

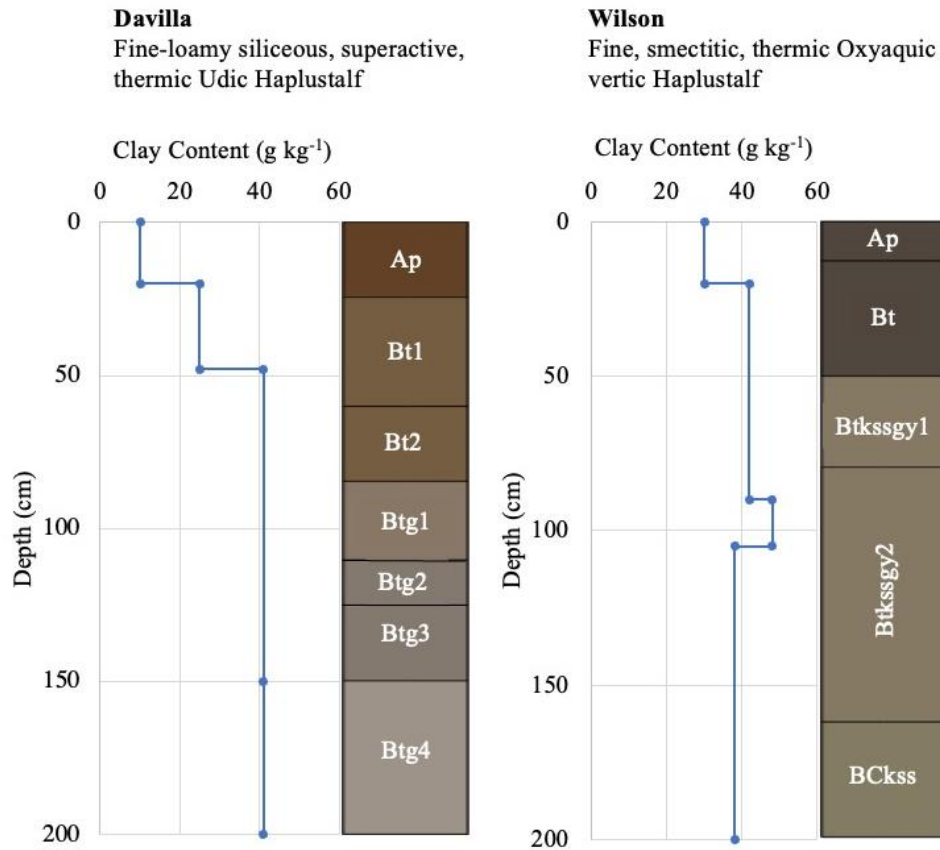


Figure 6. Average clay content with depth and horizon distinctions for Davilla and Wilson soil series (modified from Soil Survey Staff, n.d.).

Soil cores of both the Waiser and validation datasets were collected with a Giddings hydraulic soil probe (Giddings Machine, Fort Collins, CO). Each core was collected to a depth of 120 cm or the depth by which the parent material inhibited further extraction. Cores were brought back to the laboratory and refrigerated until time of scanning.

Prior to scanning, each core was cut in half, along the long edge. Each half of the soil core was scanned every 2.5 cm along the length of the cut edge. The ASD AgriSpec was used for the collection of VisNIR spectra in the 350-2500 nm range. Each 2.5-cm segment was scanned twice with a 90° rotation of the contact probe between scans. After the validation dataset cores were scanned, soil from both halves of each 2.5 cm segment was analyzed for particle size using the pipette method (Gee and Or, 2002). The NRCS field descriptions and lab-determined clay contents were used to identify horizon depths and soil properties.

The raw VisNIR spectra for all datasets were pretreated prior to model calibration and validation. Pretreatment of spectra included splicing, averaging, and converting to the 2nd derivatives of reflectance. The two replicate scans with the 90° rotation were averaged. A cubic smoothing spline was fit to each spectral curve using the R “smooth spline” function (R Development Team, 2004; Brown et al., 2006; Waiser et al., 2007).

3.2.2. Sampling for Laboratory Analysis and Classification

Because areas where the validation soil cores were collected represented complexes, VisNIR predictions of clay content along each profile were analyzed to correctly classify each soil core to the correct soil series. Although all three series have different soil textures in their A horizons, the Davilla surface texture of loam (75 to 270 g kg⁻¹ clay content) and Wilson surface texture of silt loam (0 to 270 g kg⁻¹ clay content) have overlapping clay content ranges. Predictions of surface horizon texture were,

therefore, unable to classify soils into their series. Considering the variable and unpredictable bias in predictions, it was not valuable to make further classifications based on subsurface texture or particle class size, especially without sand and silt predictions of validation data. Particle control section was then assessed as a means to categorize soils as Davilla or Wilson series. Trends regarding the prediction patterns of side-by-side, side-by-side averaged, and horizon-averaged scans were noted across both model calibrations: both intact field moist calibration and the dried ground library EPO calibration. Select whole-profile predictions of clay content were selected for several sites to report and demonstrate these trends.

3.2.3. Averaging Spectra

The validation dataset contained three further spectral averaging scenarios: (a) individual side-by-side scans, (b) averaged side-by-side scans, and (c) horizon-averaged scans. Individual side-by-side scans (a) contain VisNIR spectra taken along both halves of each core at 2.5 cm fixed depth intervals (n=1,639). Next, the VisNIR spectra at each depth on matching halves of each core were paired and averaged together (n=831) to create average side-by-side scans (b). Then, the averaged side-by-side scans were grouped by horizon and averaged accordingly (n=151) to create (c) horizon-averaged scans (Fig. 7). Additionally, averaging predictions, rather than averaging spectra, were evaluated. Predictions from side-by-side scans of the same depth (n=831) and averaged predictions from the same side-by-side scans of each soil horizon (n=151) were compared.

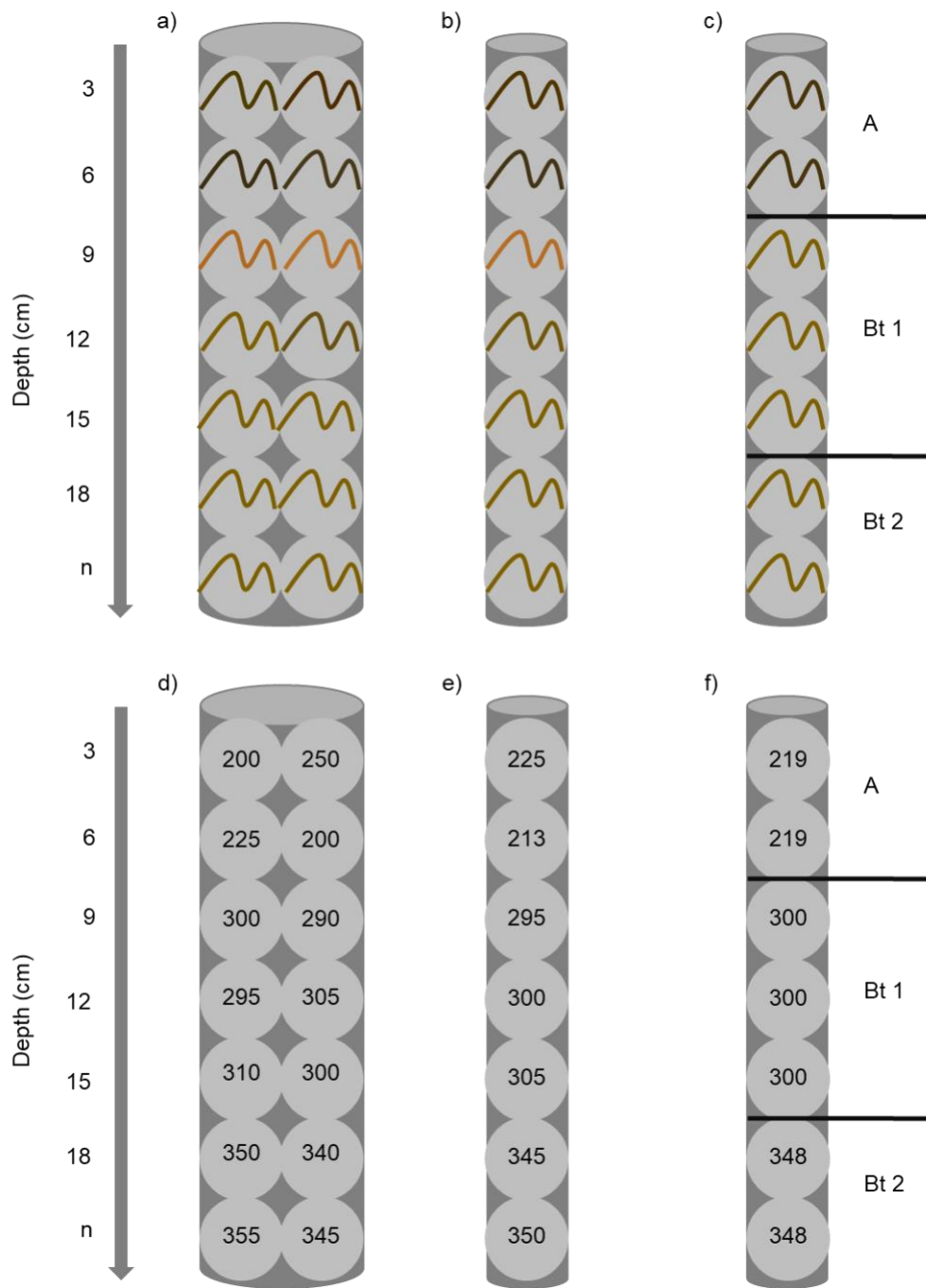


Figure 7. Schematic of VisNIR averaging: a-c depict spectra-averaged scans and d-f depict averaging of clay content predictions from VisNIR spectra (g kg^{-1}). a&d reflect side-by-side scans, b&e depict side-by-side averaged scans and c&f depict horizon-averaged scans.

The PLS models were calibrated with the number of latent variables and principle components that created the best prediction outcomes for the validation dataset, following Ackerson et al. (2016). The models calibrated with the Waiser dataset were calibrated with two natural latent variables. The models calibrated with the NRCS-Brown library and Waiser dataset EPO were modeled with two principal components and three natural latent variables. Averaging scenario (side-by-side, side-by-side-averaged, or horizon-averaged) did not impact the optimum number of variables for model calibration and prediction. All models were evaluated using three parameters to describe difference between measured and predicted values: the coefficient of determination (r^2), root-mean squared error (RMSE), and bias.

3.2.4. Soil Classification

Each soil core was classified as either a Burleson, Davilla, or Wilson series (or marked as ambiguous) by a number of methods. First, the soil map was consulted and the location of each core was used to categorize the soils. If mapped as a complex, the soil was marked as ambiguous as the map could not provide an accurate prediction of which series is present. From laboratory clay content, surface texture was predicted and marked as ambiguous if clay content fell in the overlapping clay content range (75 to 270 g kg⁻¹). Similarly, soils were classified by their laboratory measured clay content values for the particle size control sections. Surface texture and particle-size in the control section were used in combination with VisNIR predictions of clay content from horizon-averaged spectra for both modeling scenarios (Waiser calibration and NRCS

library and EPO) to classify soils once more. Due to the limitations of sand and silt to be predicted accurately from VisNIR spectroscopy, these predictions were omitted (Silva et al., 2019).

3.3. Results and Discussion

3.3.1. Intact Field Moist vs. Library and EPO Calibration

Both model calibration scenarios yielded similar accuracies for clay content predictions (Fig. 8; Table 7). For side-by-side scan predictions, the intact, field moist calibration and dried ground library with EPO calibration yielded comparable predictions, with only 5 g kg⁻¹ difference in RMSE, creating only a slight favor of the intact, field moist calibration. For the averaged side-by-side scan models, there is a slightly larger difference in RMSE (9 g kg⁻¹), although r^2 and bias are almost the same. The RSME for the intact, field moist calibration slightly out-performed the library-EPO approach. The horizon-averaged models had the largest difference in prediction parameters. The intact, field moist calibration had a smaller RMSE (52 g kg⁻¹) than the library with EPO model (66 g kg⁻¹). There was, however, a greater bias in the intact field moist calibration of 20 g kg⁻¹ compared to the library-EPO model (-6 g kg⁻¹).

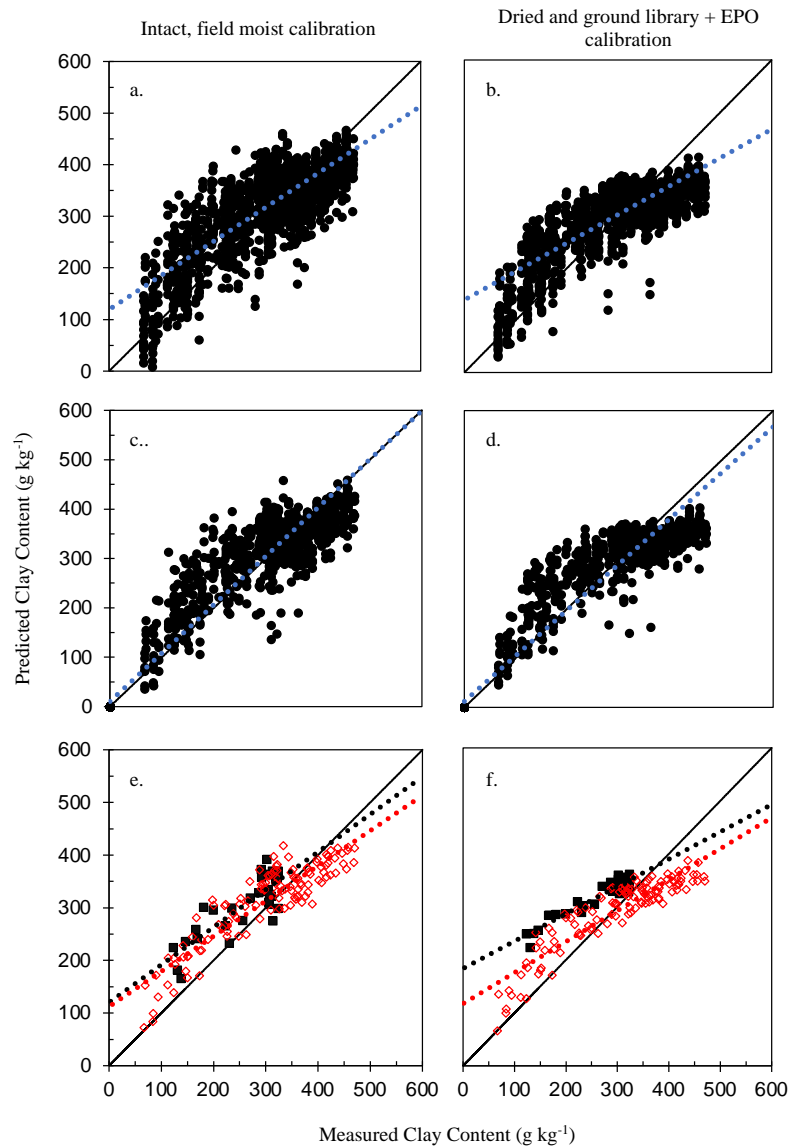


Figure 8. Measured versus predicted VisNIR predicted clay contents for moist intact VisNIR spectra using two modeling scenarios (1) an intact field moist spectral calibration model (left column) and (2) a dried ground library with an EPO projection (right column). Three validation datasets are included (a) side-by-side, (b) side-by-side averaged, and (c) horizon-averaged scans. Solid black line is a 1:1 line; in a-d dotted blue lines are fitted lines; and in e&f black dotted link indicates averaged scans from A and E horizons and red dotted line indicates Bt horizons, respectively.

In general, these results suggest a library with EPO projection provides comparable predictions to a calibration model developed using scans that include the field moist condition. Using pre-existing spectral libraries of dried ground soil scans eliminates the time and resources needed to build new *in situ* libraries that are limited in geographical scope and application by the field soil conditions in which they are collected.

3.3.2. Spectral Averaging vs. Prediction Averaging

When using the intact calibration model, neither averaging scans nor predications improved prediction accuracy. Averaging individual predictions, not spectra did improve prediction accuracy, by roughly 10 g kg⁻¹ for the library with EPO model. It must be considered that the clay content was evaluated in the laboratory for horizon-homogenized soil. We did expect the horizon-averaged predictions to yield the best accuracy because the clay measurements used for validation represented the whole horizon. It could be beneficial to have at least two VisNIR scans of each soil profile to identify where there may be a poor scan, special features, or specific characteristics in the soil. But overall, there is little difference in model performance between side-by-side scans and averaged side-by-side scans (Fig. 8, Table 8).

Table 8. Summary of prediction results for clay content from the validation dataset using the intact, field moist spectra (Waiser et al., 2007) and the dried ground NRCS-Brown library with an external parameter orthogonalization (EPO).

	Spectra Averaged			Predictions Averaged		
	r ²	RMSE	Bias	r ²	RMSE	Bias
	--g kg ⁻¹ --			--g kg ⁻¹ --		
	<i>intact calibration</i>					
Side-by-side	0.62	62	15			
Side-by-side averaged	0.65	59	15	0.67	58	15
Horizon-averaged	0.79	52	20	0.79	52	21
<i>A and E Horizon</i>	0.75	65	56	0.77	63	55
<i>Bt Horizon</i>	0.64	48	11	0.62	49	11
	<i>dried ground library + EPO calibration</i>					
Side-by-side	0.66	67	-14			
Side-by-side averaged	0.65	68	-14	0.67	58	2
Horizon-averaged	0.74	66	-6	0.74	56	7
<i>A and E Horizon</i>	0.65	72	6	0.65	71	59
<i>Bt Horizon</i>	0.62	51	-7	0.61	52	-8

3.3.3. Prediction Accuracy and Soil Horizons

The clay predictions for subsurface B horizons were more accurate than surface A horizons (Fig. 8c, Table 8). This trend held for both the intact and field moist as well as the library with EPO model. Both models for both spectral and prediction-averaged scenarios had a consistent positive bias for the A horizon (~55 g kg⁻¹). While little bias was present for the B horizon, the accuracy was around 50 g kg⁻¹.

The bias and inaccuracy in A horizon clay content predictions could be due to several factors including higher variation in moisture, lack of homogeneity at the surface, or variations in organic matter content. Ackerson et al. (2017) showed two soil profiles with accurate clay content predictions in surface horizons with low clay content (100 g kg⁻¹). While there are few pieces of evidence for clay content prediction accuracy

changes with depth, Hummel et al. (2001) found that organic matter was better predicted at the surface than in subsurface B horizons. Wijewardane et al. (2016a) reported that A horizon predictions of organic carbon had greater RMSE and lower r^2 values, but similar biases to predictions of E and B horizons. Kusumo et al. (2010) attributed the influence of roots in upper soil horizons to less accurate spectral measurements, which is perhaps another influence on this dataset.

3.3.4. Classification of Soil Series

VisNIR predictions of clay content were used for series classification by soil map and post-collection properties to assess the capabilities of VisNIR to predict soil series from predicted clay content. The limiting factor for the prediction of soil series from VisNIR predictions of clay content is the overlapping clay content ranges in soil textures at the surface. Because the textures among the three series overlap in clay content, VisNIR cannot distinguish specific textures clearly due to the lack of clay and silt information that would further classify the texture (Table 9). The particle control section was better able to categorize soils into a series classification (Davilla having fine-loamy (<350 g kg⁻¹ clay content); Wilson having fine (>350 g kg⁻¹ clay content).

Table 9. Soil classification for each highlighted soil profile by the Web Soil Survey map, laboratory data, and spectral data.

Soil profile (reference for Fig. 9)	Classification			
	Web Soil Survey Soil Map	Lab Data	Spectral Data	
			Waiser Calibration	Library + EPO
a	Wilson-Davilla complex	Wilson	Wilson	Davilla
b	Wilson-Davilla complex	ambiguous	ambiguous	ambiguous
c	Wilson-Davilla complex	Davilla	Davilla	Davilla
d	Burleson	Davilla	Wilson	Davilla

An advantage of using VisNIR spectroscopy to scan soil profiles is a resulting image of clay content throughout the profile. Figure 9 presents a selection of a VisNIR-predicted clay profile for each of the soil series investigated in the project. When all profiles were viewed, no clear trends in bias or accuracy were found among the model calibration types or soil series association. For the soil scanned in this project, clay content predictions differed from measured values up to 100 g kg⁻¹ as shown Fig. 9d. For this soil, the VisNIR prediction misses the 100 g kg⁻¹ increase in clay content at 10 cm depth. This error could lead to inaccurate classification of this soil because the argillic horizon does not clearly present in Panels b and c.

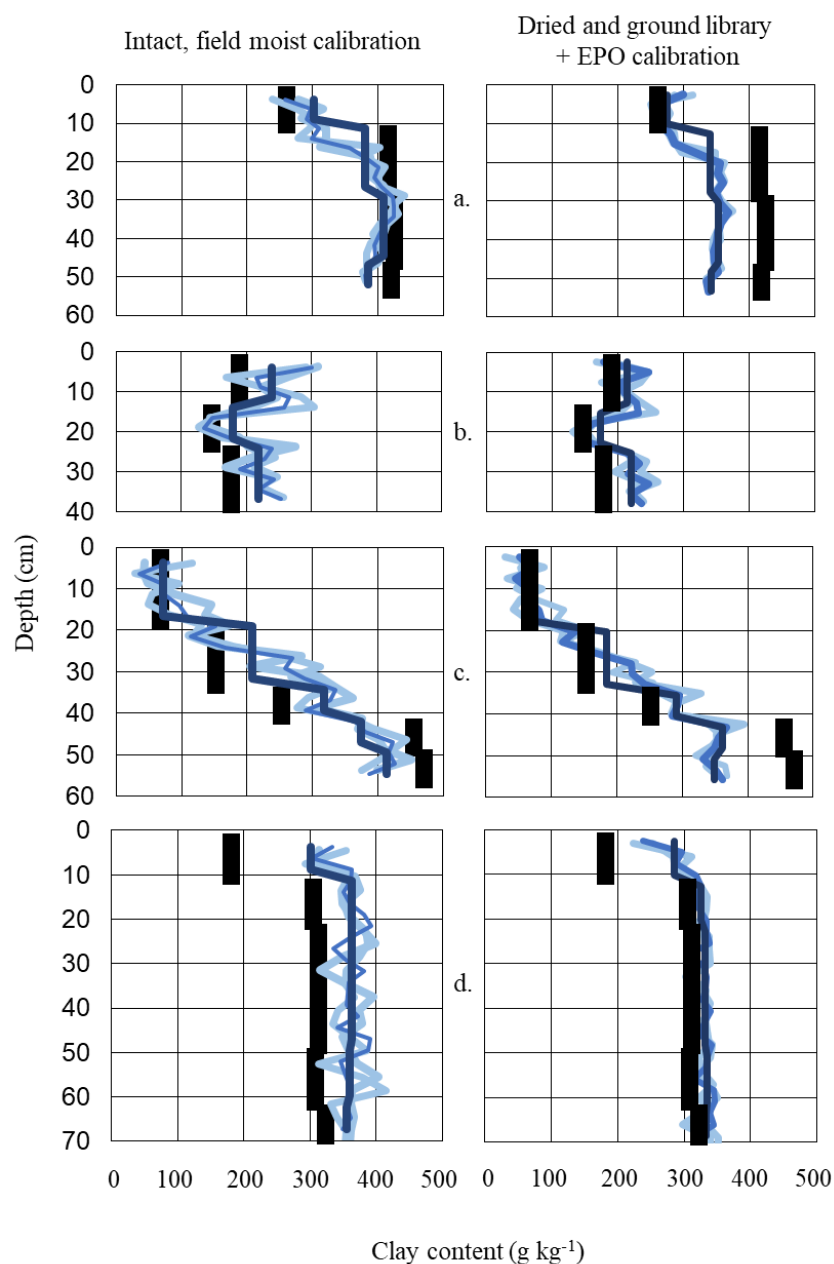


Figure 9. Whole-profile VisNIR predictions of clay using the 1) intact, field moist calibration (left panels) and 2) the dried ground library with external parameter orthogonalization (EPO; right panels). Each row of panels depicts a soil core from row a, b, c, and d in Table 9. Black bars indicate laboratory data for horizon-homogenized samples. Blue lines indicate VisNIR predictions of clay content. The two lightest lines indicate each side-by-side scan, next darkest line indicates side-by-side averaged predictions, and darkest blue line reflects horizon-averaged predictions.

The Burleson soil series is a Vertisol that requires greater than 400 g kg⁻¹ clay content throughout the whole profile. Although several sampling locations were mapped as Burleson, no soil profiles were characterized as Burleson as none met the high clay content requirement (from laboratory data or VisNIR predictions). Distinguishing between the Wilson and Davilla series was unsuccessful without careful lab data on soil texture (sand and silt in addition to clay content) because of the overlap in clay content ranges for their respective textures (70 to 270 g kg⁻¹), however, the particle size class was better able to classify soils into Davilla or Wilson series.

The soil map was unable to classify any soils into a series. Soils predicted to be Burleson did not meet the clay content requirements and all others were mapped as the Wilson-Davilla complex. Laboratory data The field moist intact calibration model classified 19 out of 32 cores as the same series as laboratory data. The library and EPO model classified soils as the same series as laboratory data for 22 out of 32 cores (Table 10). The two models predicted the same series for 21 out of 32 cores. A more specific discussion is to follow of selected soil profiles to more closely illustrate the efficacy of clay content predictions to assign soil series.

Table 10. Counts of soil series classification for soil cores as distinguished by soil map or particle control section as determined by laboratory data or VisNIR predictions of clay content.

Classification Method	Soil Series Classification			
	Burleson	Davilla	Wilson	Other
Soil Map	3	0	0	29
Laboratory Data	0	20	9	3
VisNIR Predictions:				
Field Moist Intact	0	20	12	0
Calibration				
VisNIR Predictions: NRCS-				
Brown library + EPO	0	28	2	2

One profile (Fig. 9a; Table 9a) is mapped as a Wilson-Davilla complex, classified by laboratory data as a Wilson, and was not successfully classified by VisNIR data. As with all soil cores in this data set (Table 9), VisNIR data was unable to predict surface horizon texture class by clay content alone. Laboratory data reflected 420 g kg⁻¹ clay content in the control section, classifying the soil as a Burleson or Wilson series. The VisNIR prediction indicated much less than 400 g kg⁻¹ at the surface, resulting in classification as a Wilson. The spectral predictions using the field moist intact calibration classified the soil as a Wilson, while the library with EPO predicted clay content to be under the 350 g kg⁻¹ threshold, reflecting the Davilla soil series.

A second profile (Fig. 9b; Table 9b) is mapped as a Wilson-Davilla complex and laboratory data was not useful to classify. Laboratory clay content was lower than the fine-loamy particle size class for Davilla series (and therefore lower than Wilson series). The VisNIR data were also unable to classify this soil because of the lower predicted clay content than the mapped and presented series. Likely this soil core is a variant and belongs to an unmapped series.

The third selected profile (Fig. 9c; Table 9c) is mapped as a Wilson-Davilla complex and classified using laboratory data as a Davilla series. Both VisNIR clay content prediction models successfully classified the soil as a Davilla series using the particle control section.

The fourth selected profile (Fig. 9d; Table 9d) is mapped as a Burleson and classified using laboratory methods as a Davilla series. The VisNIR data was inconclusive for this profile. Although VisNIR predictions of clay content were similar for both the intact field moist calibration and library and EPO calibration, clay content was predicted slightly above and below the 350 g kg⁻¹ threshold, respectively, favoring a Wilson series for the intact, field moist calibration and Davilla series for the library and EPO calibration.

For 10 out of 32 cores, the VisNIR predictions of clay content between the two models (intact, field moist calibration and library and EPO calibration) did not characterize the soils as the same series, both models were often predicting clay content within 50 g kg⁻¹ of laboratory values with several 10 or 20 g kg⁻¹ above or below the 350 g kg⁻¹ threshold for the particle size control section limits (Table 10). The lack of

supplementary soil properties (e.g., color, sand and silt contents, presence of clay films, carbon content, etc.) prohibited more accurate and holistic classification of these soil cores into series. Although we cannot say with absolute certainty that VisNIR predictions of clay content correctly categorized these soils into the correct series, having proximal soil sensor predictions alleviates the inputs required for traditional soil taxonomic classification, and still provides useful soil data.

Although there is a lack of literature of soil classification from spectral predictions of clay content, many have used VisNIR spectroscopy to classify soils by other properties or by other methods. VisNIR spectroscopy has been successful in identifying carbonate horizons without lab chemistry (Acree et al., 2020). Similarly, Terra et al. (2018) was able to classify soils from pedogenic properties deduced from clustering of spectra and soil characterization analysis. Demattê and Terra (2013) used a different approach, inspecting reflectance intensity and absorption features for the prediction of clay mineral contents. They were successfully able to distinguish different soils along a toposequence from this analysis. Other methods of analysis such as PLS and least discriminant analysis (LDA) may be helpful as well. Wilke (2010) was able to classify these soils with more success into their series from the pairing of the PLS model and LDA to group soils into series by their spectra and spectral properties alone, disregarding clay content predictions.

For future applications, having whole-profile clay content predictions may be useful to find horizon boundaries, where clear shifts in clay content occur for root zone or construction purposes, or perhaps to distinguish between series at finer resolutions

than what soil maps currently provide. Soil spectroscopy is, however, more accurate and provides perhaps more useful insight as to soil properties than, for example, a soil map where series distinctions often cannot be made. If assessing soil texture as a means to distinguish two series, it may be challenging if both series contain a loam, for example, with the same range of clay without sand and silt estimations to accurately assign soil texture. Particle control section was much more useful to categorize these soils than soil texture by means of VisNIR predictions of clay content.

3.4. Conclusions

Two different calibration models were used to convert intact and field moist VisNIR measurements into predictions of clay content along a soil profile. Both calibration data sets, a field a moist intact dataset, as well as, a dried ground library with an EPO transformation both predicted clay content with similar accuracies. The dried ground library with an EPO transformation more consistently resulted in less prediction bias. Averaging spectra by depth or by horizon did not significantly impact the accuracy off the clay content prediction. Having side-by-side scans or replicate VisNIR scans for each site may be of benefit to identify outliers or unusual features that may only be reflected in small sections of soil (e.g., redoxomorphic features, gypsum, etc.). Predicting clay content from averaged spectra and averaged clay content predictions with depth was equally successful. VisNIR predictions of clay content were better able to categorize soils into series than laboratory data and soil map predictions of series.

Although VisNIR spectroscopy cannot provide thorough soil taxonomic classification due to the inability to measure properties such as the presence of clay films, horizon boundaries, etc., it may be a time and cost-efficient tool to distinguish better field boundaries between series or provide crude estimates of classification into series.

4. CONCLUSIONS

In regard to uniformity in methodology, there was no conclusive evidence suggesting that the method of SOC measurement in the laboratory impacted model performance. Results suggested that using different models of spectroradiometers impacted predictions of clay and SOC. When predicting soil characteristics on dried ground soil spectra, the choice of library influences the prediction performance of SOC more than clay content. All libraries performed well and were capable of predicting both soil properties; soil spectral libraries were interoperable for dried ground spectra. When predicting soil characteristics on *in situ* spectra, the choice of dried ground library seemed to be more impactful than the choice of EPO projection dataset. The Texas EPO dataset was the most robust and was generally successful for all libraries. Visual removal of spectral outliers from replicate scans at the same depth removed few spectra, although perhaps an automation of spectral inspection may improve efficiency in future spectral analyses. Having more spectral replicates did not significantly improve prediction of clay or SOC, but may be helpful to identify outliers in spectral data. Further research may compare the ability of broad libraries and localized libraries to predict soil properties on the whole-farm level, or perhaps across a county to test how similar a predicted dataset must be for accurate model calibration. Furthermore, continued investigation of *in situ* soil property prediction with VisNIR is needed with data collected by the VisNIR-penetrometer to test the instrumentation and its ability to make real-time soil property predictions. Two different calibration models were used to

convert intact and field moist VisNIR measurements into predictions of clay content along a soil profile. Both calibration data sets, a field a moist intact dataset, as well as, a dried ground library with an EPO transformation both predicted clay content with similar accuracies. The dried ground library with an EPO transformation more consistently resulted in less prediction bias. Averaging spectra by depth or by horizon did not significantly impact the accuracy of the clay content prediction. Having side-by-side scans or replicate VisNIR scans for each site may be of benefit to identify outliers or unusual features that may only be reflected in small sections of soil (e.g., redoxomorphic features, gypsum, etc.). Predicting clay content from averaged spectra and averaged clay content predictions with depth was equally successful. VisNIR predictions of clay content were better able to categorize soils into series than laboratory data and soil map predictions of series. Although VisNIR spectroscopy cannot provide thorough soil taxonomic classification due to the inability to measure properties such as the presence of clay films, horizon boundaries, etc., it may be a time and cost-efficient tool to distinguish better field boundaries between series or provide crude estimates of classification into series.

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