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## Laboratory evaluation of two VNIR optical sensor designs for vertical soil sensing

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**Abstract.** Visible and near infrared reflectance spectroscopy (VNIR) is becoming an extensively researched technology to predict soil properties such as soil organic carbon, inorganic carbon, total nitrogen, moisture for precision agriculture. Due to its rapid, non-destructive nature and ability to infer multiple soil properties simultaneously, engineers have been trying to develop proximal sensors based on the VNIR technology to enable horizontal soil sensing and mapping. Since the vertical variation of soil properties are equally important as the lateral variation for precision agriculture decisions, VNIR can be utilized to develop sensors for vertical soil sensing as well. The objective of this study was to evaluate the performance of two VNIR probe designs using an independent soil VNIR library for model calibration. We developed and tested two designs (referred to as D1 and D2) One hundred and fifty Nebraska soil samples were randomly selected from the USDA-NRCS-KSSL soil archive and scanned by the two VNIR probes. Same soil samples were also scanned by ASD's mug lamp accessory as the standard laboratory scans. The spectra obtained from the VNIR probes were compared with standard mug lamp scans. A soil library of 1595 sample scans was used to calibrate models using partial least squares regression (PLS) for total carbon (TC), organic carbon (OC) and total nitrogen (TN). The models were used to predict for the scans obtained from D1 and D2 and the mug lamp to evaluate the performance of the designs. Results showed that, in general, both D1 and D2 followed the mug lamp scans with D1 having higher noise levels at the beginning and end of the spectrum as compared to D2. The comparison of predictions suggested that D2 performs comparably to the standard mug lamp; whereas D1 fails to achieve such accuracy due to its inherent noises in scans. Overall performance of D2 suggested its ability to be integrated into a hydraulic penetrometer for high resolution vertical soil sensing.

**Keywords.** Visible and near infrared reflectance spectroscopy, soil VNIR penetrometer, vertical soil sensing, soil organic carbon, total nitrogen, total carbon.

## Introduction

The demand for high resolution 3D soil data is increasing for many disciplines such as precision agriculture, hydrological and ecological modeling, climate modeling, and land resource management. Digital soil mapping is the sub-discipline of soil science which provides 3D quantitative soil data across different scales utilizing traditional and modern soil measurement and inference methods (Minasny and McBratney 2016). However, financial constraints usually restrict intensive sampling at higher densities, which leads to the employment of different sensing technologies (de Gruijter et al. 2010; Rossel and McBratney 1998). Researchers around the world are trying to develop more accurate and efficient soil sensors to detect different soil properties using different sensing technologies (Adamchuk et al. 2004; Hummel et al. 1996; Sudduth and Hummel 1993).

There are different sensing technologies used by soil sensing community including satellite remote sensing (Barnes et al. 2003; Ben-Dor 2002), on-the-go soil sensors (Adamchuk et al. 2004), apparent electrical conductivity/resistivity (Corwin and Lesch 2003), ground penetrating radar (Han et al. 2016; Iwasaki et al. 2016),  $\gamma$ -ray sensor (Egmond et al. 2010; Iwasaki et al. 2016; Triantafilis et al. 2013) and visible and near infrared sensors (Christy 2008; Hummel et al. 2001; Kodaira and Shibusawa 2013). They are widely used to capture the lateral variability of soil characteristics and the technologies to characterize soil profiles without pulling a soil core or opening a soil pit are still limited (Hartemink and Minasny 2014).

Visible and near infrared (VNIR) spectroscopy has some advantages over other sensing technologies such as non-contact and non-destructive nature of sensing, ease of miniaturization for a VNIR sensing probe and the ability to derive multiple soil properties using one scan. There have been numerous efforts to develop sensors based on VNIR for deriving horizontal soil properties such as organic carbon, moisture, texture, etc. (Christy 2008; Hummel et al. 2001; Kodaira and Shibusawa 2013; Mouazen et al. 2007). However, lateral soil sensing does not provide adequate inputs to cater the demand of high resolution 3D soil data for different disciplines, which creates a need to develop vertical soil sensors.

Several researchers tried to simulate vertical soil sensing by retrieving soil cores from the fields and scanning at fine vertical resolution. Hummel et al. (2001) obtained 48 soil cores from Illinois and scanned at 2.5 cm vertical resolution in six moisture levels to predict soil organic matter and moisture. Waiser et al. (2007) and Morgan et al. (2009) utilized 72 soil cores collected from Texas to conduct a simulated profile characterization of clay and soil organic and inorganic carbon. Doetterl et al. (2013) demonstrated the simulated high vertical resolution (3 cm) soil organic carbon assessment with 151 soil cores retrieved from central Belgium. In addition to laboratory simulated vertical VNIR sensing, in situ vertical soil sensing also sporadically reported in the literature. Custom-made spectral head device that can penetrate into the subsoil of a drilled hole by Ben-Dor et al. (2008), commercial Veris P4000<sup>TM</sup> probe (Veris technologies Inc., Salina, Kansas, USA) for the measurement of soil texture and organic matter (Wetterlind et al. 2015) are some example scenarios. Poggio et al. (2015) evaluated the optical performance of a newly developed VNIR foreoptic under laboratory conditions using 389 milled and pressed surface and obtained comparable results to standard ASD contact probe.

In this paper, we reported the testing of two newly developed VNIR probes in the lab. The long term goal of the authors is to use these VNIR probes to develop an integrated system for in situ high resolution vertical soil sensing. The specific objective of this study was to evaluate the performance of the two VNIR probe designs using an independent soil VNIR library to calibrate models. This particular effort was to mimic the practical application of such a sensing system where an independent VNIR library is most likely to be used for model calibrations to reduce cost constraints and achieve higher accuracy comparable to standard ASD MugLite scans.

## Materials and Methods

### VNIR library and soil samples

The spectral library used for model calibration in this study was extracted from Rapid Carbon Assessment (RaCA) Project which was initiated in 2010 by the Soil Science Division of USDA-NRCS. This was national-wide effort to capture the baseline soil carbon stocks across the conterminous U.S (CONUS). RaCA used a multi-hierarchical design to ensure that samples were evenly distributed across regions based on major land resources areas (MLRA) and land use land cover classes (LULC). A detailed description of the sampling design of the project can be found in Wills et al. (2014). A subset of RaCA samples from RaCA Region 5 was used as the library. This give a total of 1595 samples, all having the full characterization of Organic Carbon (OC), Total Carbon (TC), and Total Nitrogen (TN), as well as the VNIR reflectance spectrum of dry ground samples. All VNIR spectra were collected with an ASD Labspec<sup>®</sup> spectrometer and its MugLite accessory in the lab setting.

One hundred and fifty air-dried and ground soil samples archived at National Soil Survey Center of USDA-NRCS were extracted and used for the performance assessment of the VNIR probes. Three criteria were employed for sample selection from the archive. First, the geographic region of the samples should be from Nebraska, USA. This matches with the RaCA Region 5 of the soil library used from model calibration. Second, the samples should have the measurement of OC, TC, and TN (again, to be consistent with the library). Since OC was an emphasis property, the third criterion was used to select the samples representing the full range of OC in the archive through a 20-stratum stratified random sampling.

**Table 1. Summary statistics of soil Organic Carbon (OC), Total Carbon (TC) and Total Nitrogen (TN) for the library and the sample set used in the lab testing of the VNIR probes.**

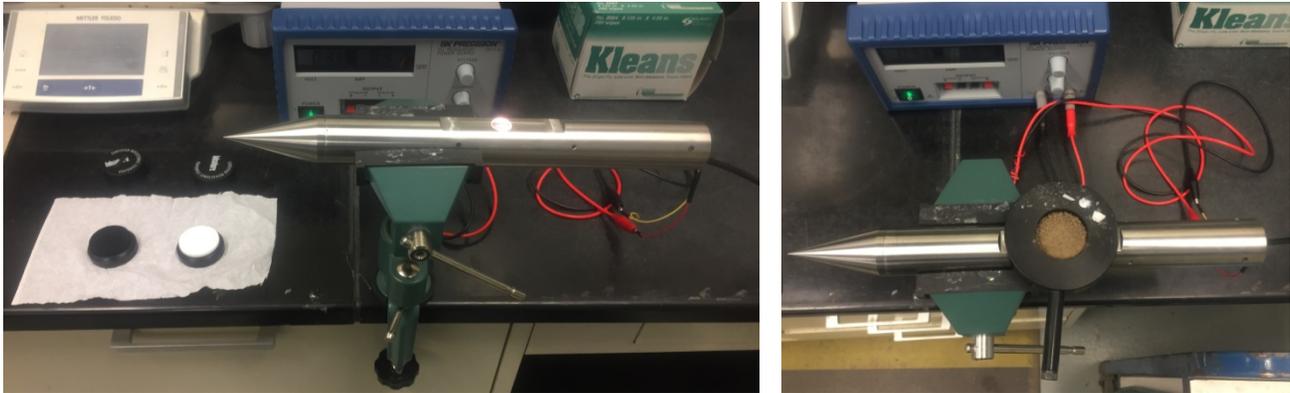
Dataset	No. of samples	Spectra measured by	Soil property	Min.	Median	Mean	Max.
Library	n = 1595	MugLite	OC (%)	0.00	0.93	1.48	38.96
			TC (%)	0.01	1.21	1.84	38.96
			TN (%)	0.00	0.12	0.17	3.09
Sample set	n = 150	VNIR probes	OC (%)	0.00	0.83	1.11	9.21
			TC (%)	0.01	1.03	1.31	10.67
			TN (%)	0.00	0.11	0.14	0.76

The library contains the samples from Region 5 of the Rapid Carbon Assessment Project.

### Laboratory testing of VNIR probes

Two VNIR probes were developed to be tested in this study. First probe (D1) consisted of an angled fiber optic cable with light source outside; while the second probe (D2) consisted of a light source and a mirror inside. The detailed information regarding the design of the two VNIR probes are not presented here due to the proprietary reasons.

The testing of VNIR probes was conducted at the Kellogg Soil Survey Laboratory of USDA-NRCS and Figure 1 shows the experimental setup. Probes were mounted on a table with the viewing aperture pointing upwards using a vise clamp to hold their position and orientation tightly. Since D2 used a halogen lamp as the light source, a DC power supply was used to provide a constant 1.0 ampere electric current with approximate 3.8 V supply voltage. For D1, SLS201 - compact stabilized broadband light source (Thorlabs Inc., Newton, New Jersey, USA) was used as the light source. Reflected light energy from the probe was acquired by an ASD LabSpec® spectrometer through the fiber optical bundle. Pucks with soil samples were then placed on the top of the viewing aperture of the probe for scanning. This configuration is similar to standard soil spectra acquire by ASD MugLite® attachment where light goes through two layers of fused silica windows between the samples and the receiving fiber optics. However this is slightly different from the intended field application since there will only be one layer of silica window (only the window of the probe).



**Fig 1. Laboratory experimental setup for the testing of the VNIR probes**

A standard Spectralon panel with 99% reflectance (Labsphere Inc., North Sutton, NH, USA) was used as the white reference in 10 minute intervals to ensure proper calibration of the spectrometer. Additionally, a standard dark reference panel with 2% reflectance (Labsphere Inc., North Sutton, NH, USA) was used to acquire the internal light back scattering of the probes. All acquired spectra from D1 and D2 were corrected as shown in Equation 1.

$$R_{DRC} = \frac{E_s - E_{DR}}{E_{WR} - E_{DR}} \quad (1)$$

where  $R_{DRC}$  is the dark reference corrected (DRC) reflectance of the sample,  $E_s$  is the reflected energy by the sample,  $E_{DR}$  is the reflected energy by the dark reference panel and  $E_{WR}$  is the reflected energy by the white reference panel.

The selected 150 samples were scanned with D1 and D2, and then with the ASD MugLite (ML) attachment. The original spectra consisted of wavelengths from 350-2500 nm. However, only 400-2500 nm range was used for the data analysis due to noises observed in the 350-399 nm range. All spectra including the modeling library were preprocessed with Savitzky-Golay (Savitzky and Golay 1964) smoothing with 3<sup>rd</sup> order polynomial and 11 nm window prior to the data analysis.

All the models for the different properties (i.e. OC, TC and TN) were calibrated for the modeling library ( $n = 1595$ ) using partial least squares regression (PLS). The number of latent factors ( $n_{LV}$ ) was allowed to vary from 1 to 30, and the size of a model was selected for the  $n_{LV}$  that gave the minimum  $RMSE_{CV}$  (Root Mean Squared Error of Cross Validation) with 25 random segment cross-validation. Since the spectra acquired from D1 exhibited significant noises at the beginning and end of the spectrum, PLS models were calibrated using two wavelength ranges: 400-2500 nm and 500-2300 nm (noisy region of D1 removed).

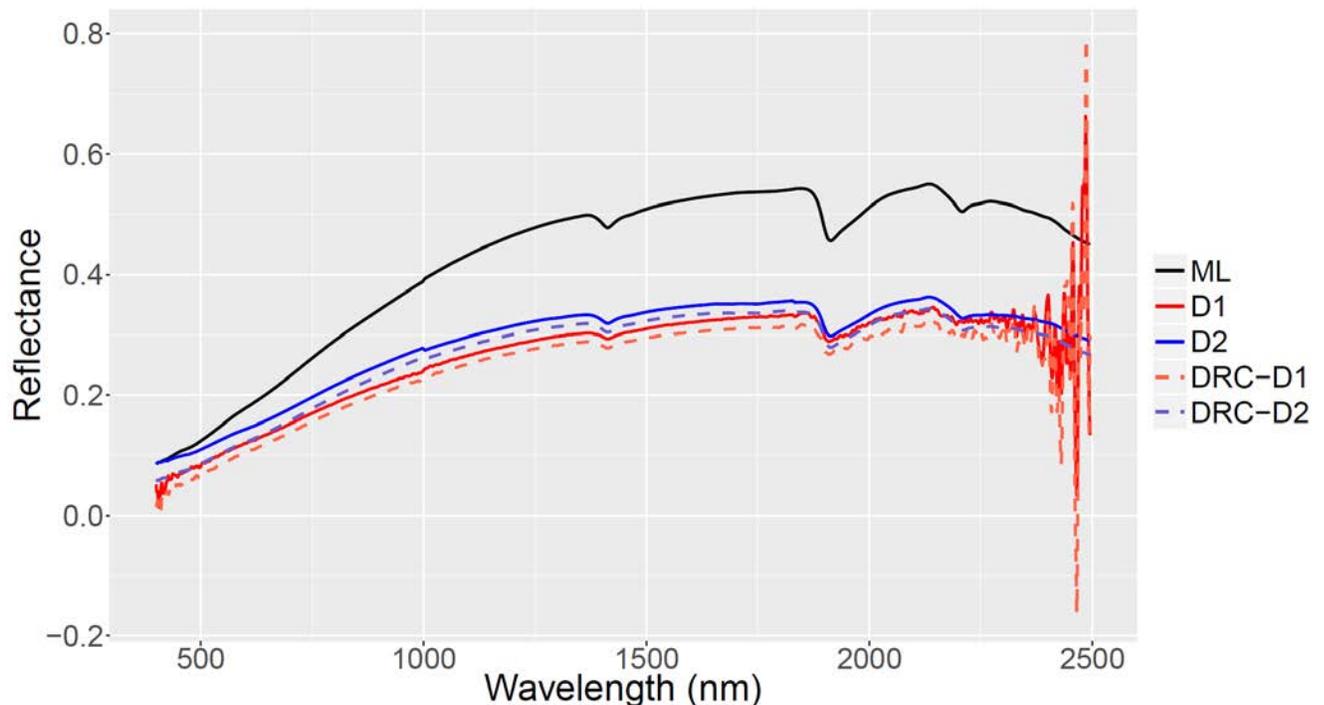
Models were used to predict different soil properties using the sample spectra acquired by D1, D2

and ML.  $R^2$  (Coefficient of Determination), Bias,  $RMSE_P$  (Root Mean Squared Error of Prediction), and RPD (Ratio of Performance to Deviation) were calculated for all the predictions to compare the performance of the designs against the standard MugLite. The data analysis was conducted in the R environment (R Core Team 2015) with packages “pls” for PLS model calibration (Mevik et al. 2013), “prospectr” for Savitzky-Golay preprocessing (Stevens and Ramirez-Lopez 2013), “caret” as the modeling wrapper (Max et al. 2015), “doParallel” for parallel processing (Analytics and Weston 2015) and “ggplot2” for graphing (Wickham 2009).

## Results and Discussion

### Spectral quality

Figure 2 shows the spectrum of one selected sample obtained from D1, D2 and ML.

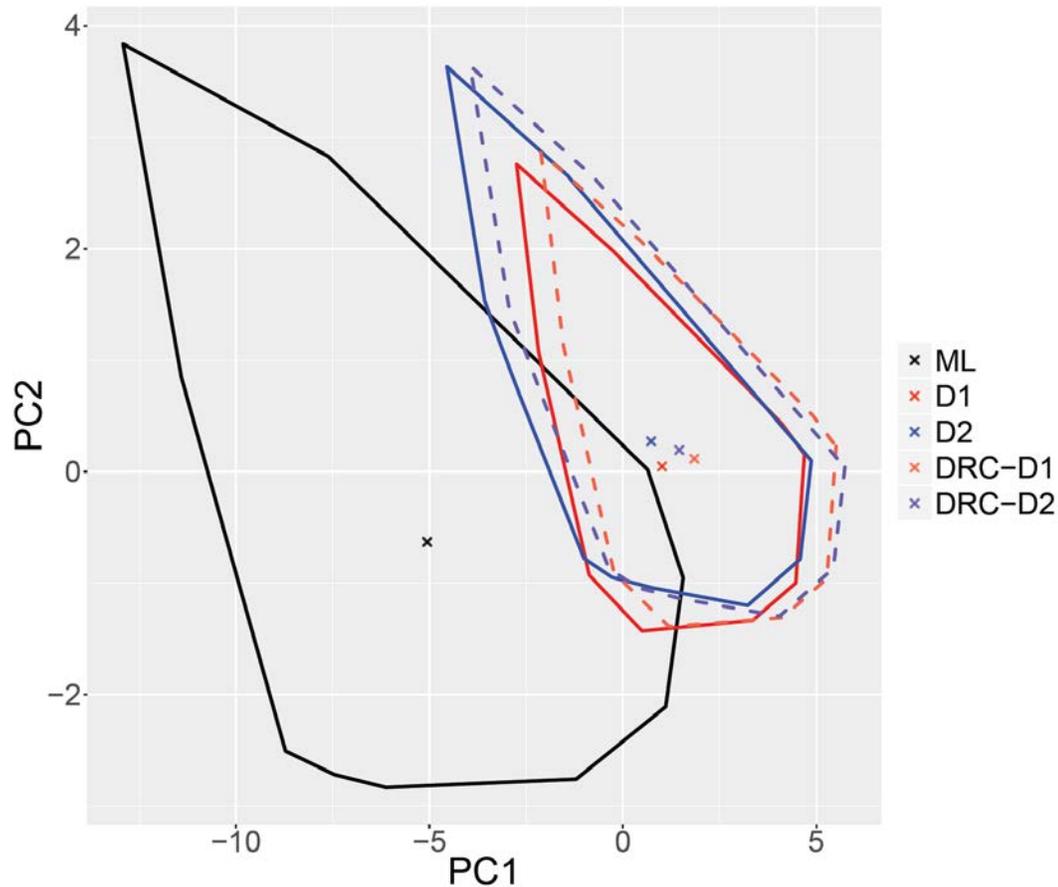


**Fig 2. Spectra obtained from VNIR probe designs D1, D2, dark reference corrected D1 (DRC-D1), dark reference corrected D2 and MugLite (ML).**

It can be seen in Figure 2 that both D1 and D2 had systematic lower reflectance throughout the entire wavelength range. This could be mainly attributed to the difference in optical configurations between the MugLite and the VNIR probes. If the soil surface acts as perfect Lambertian surface, both MugLite and VNIR probes should receive the same amount of energy at any viewing angle. However, since these soil surfaces are not Lambertian and the viewing angles of the MugLite and VNIR probes are different, VNIR probes could intercept lower reflected energy compared to MugLite. This type of systematic deviations of spectra can be corrected using spectral treatment methods such as direct standardization and piecewise direct standardization (Fearn 2001; Feudale et al. 2002; W Ji et al. 2015; Wang et al. 1991).

Dark reference correction did not affect the spectra significantly, suggesting lower internal scattering (<2%) in the VNIR probes. According to Figure 2, it was evident that D1 had higher noises at the beginning (400-499 nm) and end (2301-2500 nm) of the wavelength range. This could be due to the optical characteristics of the custom made bifurcation cable used in D1 restricting sufficient energy throughput at lower and higher wavelength regions. Unlike D1, D2 showed smooth spectra

analogous to ML spectra throughout the whole wavelength range. This suggests satisfactory optical configuration of D2 in comparison with ML. Since the noise free wavelength range for D1 was 500-2300 nm, convex hulls using all the spectra with 500-2300 nm were plotted in PC space for different scanning sources to evaluate their overall spectral discrepancies (Figure 3).



**Fig 3. Convex hulls for all spectra by VNIR probes D1, D2, dark reference corrected D1 (DRC-D1), dark reference corrected D2 and MugLite (ML).**

According to Figure 3, the convex hulls of the designs approximately preserved the shape of the convex hull of MugLite, suggesting the satisfactory optical performance of the designs to acquire spectra comparable to standard MugLite. However, the distance between the center of MugLite and the VNIR probes clearly represents the systematic variation of the spectra (as indicated in Figure 2 as well). The centers of the D1 and D2 were closer to the corresponding dark reference corrected spectra indicating non-significant effects of dark reference correction.

### Prediction performance of different VNIR designs

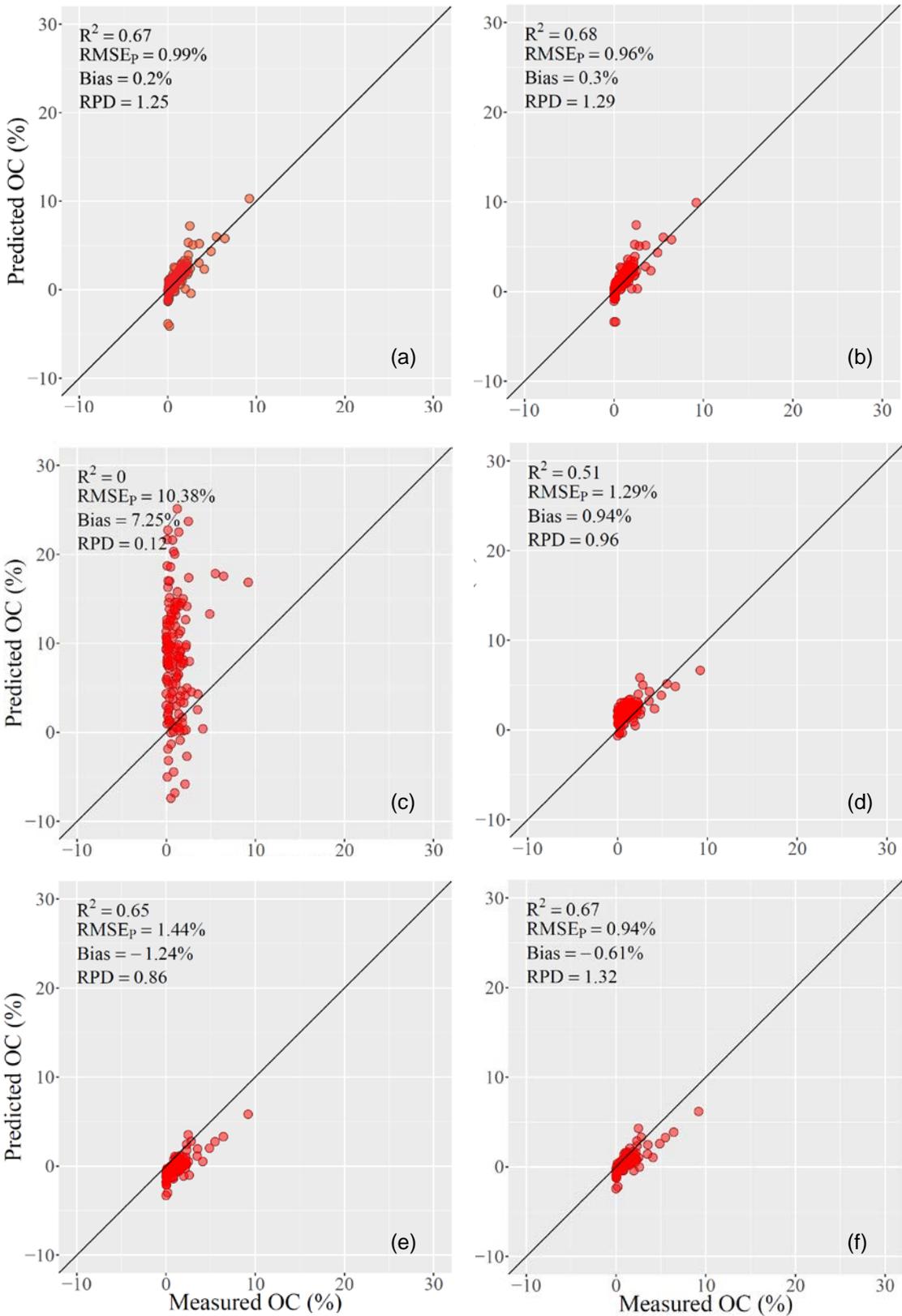
The PLS models calibrated using 400-2500 nm wavelength range had a cross-validation  $R^2$  of 0.77, 0.79 and 0.74, RMSE of 1.27%, 1.27% and 0.12%, for OC, TC and TN, respectively. Similarly, models calibrated with 500-2300 nm wavelength range had a cross-validation  $R^2$  of 0.74 for all properties with RMSE of 1.26%, 1.42% and 0.11% for OC, TC and TN, respectively. It was observed that the  $R^2$  of all models calibrated are quite similar and higher than 0.74, indicating similar and adequate model performances. Table 2 shows the prediction performance of different VNIR probes as compared to MugLite for OC, TC and TN.

**Table 2. Prediction performance of different VNIR probes as compared to MugLite for Organic Carbon (OC), Total Carbon (TC) and Total Nitrogen (TN).**

Wavelength Range (nm)	Property	Scanning source	R <sup>2</sup>	RMSE <sup>a</sup> <sub>P</sub> (%)	Bias (%)	RPD <sup>b</sup>
400-2500	OC	ML <sup>c</sup>	0.67	0.99	0.20	1.25
		D1 <sup>d</sup>	0.00	10.38	7.25	0.12
		D2 <sup>e</sup>	0.65	1.44	-1.24	0.86
		DRC-D1 <sup>f</sup>	0.02	9.35	2.55	0.13
		DRC-D2 <sup>g</sup>	0.65	1.17	-0.90	1.06
	TC	ML	0.69	1.00	0.33	1.33
		D1	0.00	49.64	22.52	0.03
		D2	0.68	1.59	-1.40	0.83
		DRC-D1	0.00	51.90	4.88	0.03
		DRC-D2	0.66	1.28	-1.03	1.03
	TN	ML	0.67	0.09	0.02	1.53
		D1	0.00	1.19	0.87	0.11
		D2	0.64	0.10	-0.07	1.28
		DRC-D1	0.00	1.01	0.32	0.13
		DRC-D2	0.63	0.09	-0.03	1.55
500-2300	OC	ML	0.68	0.96	0.30	1.29
		D1	0.51	1.29	0.94	0.96
		D2	0.67	0.94	-0.61	1.32
		DRC-D1	0.43	1.51	1.16	0.82
		DRC-D2	0.67	0.85	-0.44	1.46
	TC	ML	0.51	1.40	0.61	0.94
		D1	0.34	1.38	0.59	0.96
		D2	0.49	1.00	0.21	1.33
		DRC-D1	0.20	1.66	0.76	0.80
		DRC-D2	0.50	1.13	0.58	1.17
	TN	ML	0.67	0.09	0.03	1.52
		D1	0.54	0.15	0.12	0.90
		D2	0.65	0.08	-0.01	1.65
		DRC-D1	0.42	0.16	0.13	0.80
		DRC-D2	0.65	0.08	0.01	1.67

<sup>a</sup>Root means squared error of prediction; <sup>b</sup>Ratio of prediction to deviation; <sup>c</sup>MugLite scans; <sup>d</sup>Scans from design 1; <sup>e</sup>Scans from design 2; <sup>f</sup>Scans from Design 1 with dark reference correction; <sup>g</sup>Scans from Design 2 with dark reference correction

According to Table 2, all the predictions showed a highly varying statistics. R<sup>2</sup> and RPD varied from 0 – 0.69 and 0.03 – 1.67 respectively. When the models were applied for MugLite scans, it resulted R<sup>2</sup> >0.67 except for TC with 500-2300 nm range, indicating the applicability of the library models to the sample set selected for the study. The highest performance was always observed when the models were applied for MugLite scans since MugLite was the standard scanning source for the modeling library as well. Figure 4 shows the prediction plots for different scanning sources for OC. Though not shown here, TC and TN showed similar performances as in Figure 4.



**Fig 4. Prediction plots for scans by different scanning sources for Organic Carbon (OC). First column represents spectra for the wavelength range 400-2500 nm and second column for wavelength range 500-2300 nm. First, second and third rows indicate MugLite, D1 and D2 scanning sources respectively.**

According to Table 2 and Figure 4, it was evident that when the models were applied for the scans derived from D1 with full wavelength range (i.e. 400-2500 nm), the prediction performances were significantly decreased with very low  $R^2$  and higher RMSE<sub>p</sub>. This was mainly due to the high noises observed at the starting and end of the spectra as shown in Figure 2. However, the prediction performances were significantly increased (Figures 4c vs d), when noisy regions were removed from the spectra indicating the D1 also has the ability to be used to acquire soil VNIR spectra if the noise regions are removed.

According to Table 2, dark reference correction did not significantly affect the prediction accuracies of D1 and D2, indicating lower internal scattering of the probe designs. Figure 2 and 3 suggested that the dark reference correction did not significantly altered spectra and thus leading to similar prediction accuracies. As compared to MugLite scans, D2 and D1 with noise removed wavelength region (i.e. 500-2300 nm) showed higher bias across all the properties tested. This could be attributed to the systematic spectral shift in D1 and D2 as shown in Figures 2 and 3.

Unlike D1, D2 performed similarly across all the properties regardless of the wavelength regions used and always showed higher performance than D1. Since D2 had the ability to acquire smooth spectra along the whole wavelength region as shown in figure 2, it was able to perform comparably to MugLite and yield higher accuracies. This indicated the robustness and superiority of the VNIR probe D2 over D1 and the ability to use as a substitute for MugLite in field conditions.

### **Future work**

In this study the optical performance of two newly developed VNIR probes for soil sensing were evaluated in laboratory conditions in comparison to the standard MugLite scans. From the results it was evident that probes (especially D2) have the ability to be used in field conditions. However, field implementation of such a VNIR system for soil sensing poses a few more challenges to be addressed.

First challenge is that spectral discrepancies created by field conditions (i.e. moisture, aggregation, temperature) and global-local library variation. The laboratory spectra are usually obtained under dry ground conditions; while the field samples are highly diverse in moisture and aggregation, which can significantly affect the spectra (Minasny et al. 2011). Literature suggests different techniques such as spiking, direct standardization, piecewise direct standardization and external parameter orthogonalization could remove these external effects from spectra (Ge et al. 2014; W Ji et al. 2015; W. Ji et al. 2015; Minasny et al. 2011; Wijewardane et al. 2016).

There is a tendency to develop easily accessible large spectral libraries (Brown et al. 2006). However, spectral differences between modeling library (i.e. global) and target field (i.e. local) can pose a significant influence on the performance of the models calibrated on a global library (Guerrero et al. 2016). The global spectral library may not represent and capture the spectral variation in the local conditions, leading to poor model performance of global models in the local conditions. There are several reports in the literature to suggest that spiking can significantly improve the applicability of the models calibrated for global libraries in local conditions (Guerrero et al. 2016; Sankey et al. 2008).

The second challenge is develop a complete integrated VNIR system robust enough to different field conditions such as different soil textures, temperatures, and aggregation. This requires a durable and flexible engineering design to acquire high quality spectra comparable to laboratory spectra under diverse working environments.

The overall success of such a system depends on the careful integration of a well-engineered hardware to capture high quality spectra with low noises and software to correct for spectral discrepancies created by field conditions. Still the research question remains whether to use different layers of spectral corrections for field conditions and global-local variation or use one robust correction technique to address all the spectral differences at once. Our long term objective is to seek for the answers to this question via well-planned field evaluation of an integrated VNIR vertical

soil sensing penetrometer.

## Conclusions

In this study two VNIR probes for high resolution vertical soil sensing were evaluated under the laboratory condition. A spectral library with 1595 samples was used to calibrate models for three different properties: Organic Carbon, Total Carbon and Total Nitrogen. One hundred and fifty samples selected from Nebraska were scanned from the two VNIR probes and standard MugLite attached to ASD Labspec<sup>®</sup> spectrometer. According to the results, the D1 probe was observed with high noise at the beginning and end of spectra leading to poor performance in the predictions. However, when the noise regions were removed, D1 significantly improved the performance and resulted comparable accuracy to standard MugLite scans. Conversely, D2 probe yielded smooth spectra throughout the whole wavelength regions and obtained similar performance to MugLite. Both designs had low internal scattering. Overall D2 showed superior performance to D1. The field implementation of D2 with a complete VNIR system should be able to acquire quality spectra to enable rapid and accurate sensing of vertical soil characteristics.

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