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Research Paper

Assessment of soil properties *in situ* using a prototype portable MIR spectrometer in two agricultural fields

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Mid-infrared (MIR) soil spectroscopy has shown applicability to predict selected properties through various laboratory studies. However, reports on the successful use of MIR instruments in field conditions (*in situ*) have been limited. In this study, a small portable prototype MIR (898–1811 cm^{-1}) spectrometer was used to collect soil spectra from two agricultural fields (predominantly organic and mineral soils). Both fields were located at Macdonald Campus of McGill University in Ste-Anne-de-Bellevue, Quebec, Canada. In each of the 120 predefined field locations, *in situ* spectroscopic measurements were repeated three times and one representative soil sample was analyzed following conventional laboratory procedures. For every soil property, a field-specific partial least squares regression (PLSR) model was developed and evaluated using a leave-one-out cross-validation routine. Each soil property was evaluated in terms of the accuracy and reproducibility of model predictions. Among tested soil properties, soil organic matter, water content, bulk density, cation exchange capacity (CEC), Ca and Mg yielded higher model performance indicators ($R^2 > 0.50$ and RPD > 1.40) as compared to soil pH, Fe, Cu, phosphorus, nitrate-nitrogen, K or Na. In most instances, the error estimate representing the prediction reproducibility was found to be as high as 50% of the overall prediction error. This was due to the combination of optical and electrical noise and soil micro-variability causing soil spectra representing the same field location to yield different predictions.

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1. Introduction

Precision agriculture (PA), which is important for sustainable crop production, is becoming common practice for growers around the world. PA allows for the efficient, site-specific use of inputs (e.g. water, mineral nutrients and other chemicals) to increase farming profitability while reducing negative pressure on the surrounding environment (Gebbers & Adamchuk, 2010). To match agricultural inputs with local needs, it is necessary to understand spatial soil heterogeneity. Unfortunately, traditional soil sampling and laboratory analysis are expensive and laborious. Therefore, proximal soil sensing has been viewed as an efficient alternative that could significantly increase the affordability of soil measurements (Viscarra Rossel, Adamchuk, Sudduth, McKenzie, & Lobsey, 2011). For example, diffuse reflectance spectroscopy in the mid-infrared (MIR) range is rapid, cheap, accurate, non-polluting, and can measure a range of soil properties using a single spectrum (Viscarra Rossel, Walvoort, McBratney, Janik, & Skjemstad, 2006).

Intensive fundamental molecular frequencies are associated with soil components in the wavelength between 2500 and 25,000 nm (Janik, Merry, & Skjemstad, 1998) and show good potential for using MIR spectroscopy to predict soil properties (Soriano-Disla, Janik, Viscarra Rossel, Macdonald, & McLaughlin, 2014). For example, soil properties such as soil moisture content, soil texture, organic carbon (OC), phosphors capacity, P_2O_5, cation exchange capacity (CEC), extractable aluminum (Al), manganese (Mn) and exchangeable calcium (Ca), magnesium (Mg) were predicted using MIR spectroscopy with a coefficient of determination (R^2) > 0.5. Janik and Skjemstad (1995) predicted OC, total nitrogen, pH, sum of cations, carbonate and clay with R^2 values between 0.72 and 0.95. Qualitative description was given by identifying the soil components responsible for the correlations between the MIR spectra and soil properties. Viscarra Rossel and McBratney (2001) also suggested that soil pH and lime requirements could be predicted using MIR. A range of heavy metals, including iron (Fe), cadmium (Cd), copper (Cu), nickel (Ni) and zinc (Zn), were also predicted (except for lead, Pb) using MIR with root mean squared deviation values up to 3.3 times smaller than near-infrared (NIR) (Siebielec, McCarty, Stuczynski, & Reeves, 2004). Madari et al. (2006) found, not only carbon and nitrogen, but also clay, sand and silt as well as parameters such as soil aggregation indices can be estimated by this technology. A prediction R^2 as high as 0.97 of different carbon fractions using MIR was also reported (Janik, Skjemstad, Shepherd, & Spouncer, 2007). By summarising the results of more than 130 articles comparing the prediction of various soil attributes using the spectra of ultra violet (UV), visible, NIR, MIR or combined regions, Viscarra Rossel et al. (2006) concluded that in general, MIR produced more accurate models over other spectral ranges. However, failure to predict soil properties, including electrical conductivity, NH_4–N, NO_3–N, C/N, phosphorus, potassium, clay, silt and sand was also reported in the literature (Djuuna, Abbott, & Russell, 2013), in addition to all of the success stories. All of the studies were based on MIR spectra collected on air- or oven-dried and ground soil samples processed in the laboratory. The large size, sophistication and fragility often restrict the use of MIR technology based instruments *in situ*. Furthermore, MIR spectra are known to be easily affected by moisture and sample preparation (Reeves, 2010).

More recently, with the availability of commercial portable MIR instruments, the potential for *in situ* and real-time applications of MIR spectroscopy are emerging. Among the limited number of published reports, Linker (2008) used attenuated total reflectance (ATR), a sampling technique, to collect MIR spectra (800-1550 cm^{-1}) from 202 soil samples close to water saturation and reported a successful soil classification. Reeves (2010) used a portable Fourier transform (FT) MIR spectrometer, SOC 400 (Surface Optics Corp., San Diego, CA), to scan samples in both field moist and dry conditions. He concluded some soil properties were poorly predicted (prediction accuracy was not reported) might be due to the effect of water on the MIR spectra. Other studies used portable MIR spectrometers only on dried and ground soils. For example, Forrester et al. (2015) compared the performance of a handheld MIR instrument, Agilent 4100 spectrometer (Agilent Technologies, Santa Clara, CA, USA), to a bench-top MIR spectrometer using oven-dried and ground soil samples.

In a recent study, Dhawale, Adamchuk, Prasher, Viscarra Rossel and Ismail (2015) investigated a prototype, portable MIR variable-filter-array diffuse reflectance infrared FT spectrometer (Wilks Enterprise, Inc., East Norwalk, Connecticut, USA) to collect soil spectra in two moisture conditions. However, the spectroscopic measurements were performed on simulated moist samples, by re-wetting dried and ground soil samples. While drying and grinding change the soil physical conditions, artificially wetted soil may not behave the same way as soils from the natural conditions in a field. For example, the artificially wetted soil may not result in the uniform distribution of soil moisture as occurs in natural soils. Additionally, naturally aggregated soils have well-established pore spaces and get altered with disturbance, such as drying and grinding. The differences may have a direct effect on reflected MIR spectra. Though, the results show that this portable spectrometer was able to predict clay and sand content of mineral soil samples, its performance on more heterogeneous soils (for an example, organic soil) was inconclusive. Suitability for predicting multiple soil properties needs to be tested.

Moreover, prior MIR research has employed either one spectrum per sample or an average of several spectral scans obtained in the same position or after a slight shift of the instrument. Therefore, prior publications failed to address the reproducibility of soil spectral measurements and how reproducibility error would affect the overall prediction of targeted soil properties.

The ultimate goal of this research was to evaluate the performance of a portable MIR variable-filter-array diffuse reflectance infrared FT spectrometer in natural field conditions. More specifically, the objectives of this study were to (i) qualitatively assess the spectra collected *in situ* on naturally wet soils, (ii) predict a range of soil chemical properties including OM, pH, CEC, K, Ca, Fe, Nitrate-Nitrogen (N), Mg, phosphorus (P), Na and Cu and physical properties, including bulk density (BD), gravimetric water content (GWC) and volumetric water content (VWC), and (iii) assess the prediction reproducibility from the spectra recorded using this instrument.