



# Wet or dry? The effect of sample characteristics on the determination of soil properties by near infrared spectroscopy



J.J. Roberts, D. Cozzolino \*

School of Medical and Applied Sciences, CQIRP (Central Queensland Innovation and Research Precinct), Central Queensland University (CQU) Australia, Bruce Highway, North Rockhampton, Qld 4701, Australia

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## ABSTRACT

Most of the published articles related to the application of near infrared (NIR) spectroscopy for the quantitative analysis of soils parameters, have reported experiments or studies that are largely laboratory based where soil properties such as soil organic carbon (SOC) content are assessed on dry and sieved samples. The recent arrival of hand-held and portable analytical equipment allowing for the quantitative analysis of samples *in situ* have provided new possibilities for the analysis of soils. The implementation of this type of instrumentation will result in reduced time and cost of analysis, and will have a profound effect on the associated method steps (e.g. storing, drying, and sieving) currently used when soils are analysed in the laboratory. The aim of this short review is to highlight the gaps in the research related to the analysis of soil samples by NIR spectroscopy with high moisture (HM) content. Inconsistent results were found in the scientific literature in relation with the ability of NIR spectroscopy to measure soil chemical properties with HM content. The use of pre-processing methods did not improve the calibrations nor the selection of samples with different moisture levels. The re-wetting (hydration) of the sample and the conversion of units into volumetric ones led to optimism for the measurement of in field samples by NIR spectroscopy. However, in field applications are still in their infancy.

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## 1. Introduction

Quantification of soil parameters by near infrared (NIR) spectroscopy has become an interesting and attractive topic for research in soil science targeting several issues associated with agriculture and the environment, as reported by several authors [1–6]. Although NIR spectroscopy has been explored and used to determine

several chemical and physical properties in soils, the diversity of soil mineral composition and the low content of organic matter (OM) make their quantification by NIR spectroscopy a real challenge in routine applications of this technology [1,2].

The increasing number of publications on this topic and the worldwide incorporation of this technology by several research groups in recent years, demonstrates the growing interest on the use of NIR spectroscopy as recently reviewed by Malley and collaborators [1], Cozzolino [2], Armenta and de la Guardia [4] and Nduwamungu and collaborators [6]. More recently the possibility to develop site specific or global methods and protocols based on

\* Corresponding author. Tel.: +61 749306688; fax: +61 7 4930 6536.  
E-mail address: [d.cozzolino@cqu.edu.au](mailto:d.cozzolino@cqu.edu.au) (D. Cozzolino).

NIR spectroscopy have been expanded due to the inherent characteristics and properties of this methodology (e.g. non-destructive, rapid, low cost) [1–6]. However, several issues are still not solved or even fully understood when soil samples having high moisture (HM) levels are analysed using NIR spectroscopy. One example is the identified need to gather international data sets from different soil origins to provide reference methods which are correctly aligned (e.g. same analytical protocols, sampling strategies, etc.) with the results derived from the NIR calibration in order to make them comparable [7]. Another important issue is related to the analysis of soils with HM levels or in field soil samples, mainly because the body of knowledge in the field of soils and infrared (IR) spectroscopy is based on the use of dry and ground samples [1–6].

In recent years the increasing use of hand-held or portable IR instruments, and the development of new algorithms or the increasing use of chemometrics have changed the way the IR spectroscopy is used to measure different properties in soils. The aim of this short review is to highlight the gaps in the research related with the analysis of soil samples with HM content by NIR spectroscopy.

## 2. Laboratory, hand-held and on the go instruments to measure soil properties

Most of the published studies related to the application of NIR spectroscopy for the quantitative analysis of soil properties are focused on experiments or studies that are largely laboratory-based, with soil properties such as soil organic carbon (SOC) content assessed on dry and sieved soil samples [1–6].

The recent arrival of hand-held and portable analytical equipment allowing for the quantitative analysis of samples *in situ* has provided new possibilities for the analysis of soil samples. The incorporation of this type of instrumentation into the routine analysis of soils will result in a reduction in the time and cost of analysis currently needed. Additionally, it will have profound effects of the associated method steps (e.g. storing, drying, and sieving) currently used when samples are analysed in the laboratory. Furthermore, the use of these instruments will also reduce method error and advantageously assesses soil properties in the environment in which it belongs [8–12].

In recent years, the so called in field/on the go visible (VIS) and NIR spectroscopy for the analysis of soil samples have shown particular promise, with a significant increase in research activity with a number of applications and reports found in the literature in relation to this topic [11–13]. According to these studies, the main objective for the use of VIS-NIR spectroscopy in the field was to collect a unique reflectance spectrum from a soil where the reflectance at each wavelength is dependent on vibrational frequencies of molecules containing carbon and other soil properties [14,15].

Nowadays, different commercially available VIS-NIR and mid infrared (MIR) instruments (hand-held, portable) provide the capability of collecting spectra using either the whole or part of the electromagnetic spectrum in the VIS and NIR wavelength range between 400 and 2500 nm [16–21]. The availability and development of fiber optic cables attached to a light source allowing the collection of the spectral information from the sample utilising different detectors (e.g. GaAs diode-array, Si array) is another common setup extensively used the field [16–23].

## 3. Chemometrics is not always the answer

As in many applications associated with NIR spectroscopy, different chemometric techniques are commonly used to process the spectra and then develop prediction models for a specific or groups of properties in the soil sample analysed [24,25]. For example, several studies reported that different pre-processing techniques can provide

a specific way to increase the signal-to-noise (S/N) ratio of the data collected [25,26]. It has also been reported that wavebands exhibiting obvious noise (often at the extremes of the measurement range) might be excluded during calibration and the spectra smoothed using the Savitzky-Golay algorithm [25].

Selection of the calibration method and its performance in modelling reflectance spectra is one of the main factors for calibration success [26]. However, in most of the NIR applications, the different pre-processing methods or techniques and algorithms that might be used to develop a calibration model depend on the corresponding spectral interaction of the predominant soil chromophores [27,28]. In recent years, several authors attempted to improve SOC and clay calibrations using fused sensor data approaches [29]. However, despite good correlations, the individual calibrations for SOC and clay based on spectral data were inferior to those based on fused data. These authors concluded that the presence of water in the soil matrix affects the NIR spectrum of the soils samples [29].

However, the application and use of pre-processing techniques or algorithms by several researchers in the field of soil analysis using NIR spectroscopy did not improve the models developed for the measurement of different properties in soils [26–29]. This is even more evident for the prediction of chemical properties from wet or in field soil samples using NIR spectroscopy [26–29].

## 4. Soil chromophores and the NIR spectrum

The potential use of NIR spectroscopy to predict organic compounds in soils, and in particular SOC, has been extensively evaluated and reviewed by several authors [1–6]. However, few studies can be found on the basic understanding or the core principles governing the measurement of soil properties using NIR spectroscopy. Most of the reported calibrations were considered poorer than many researchers anticipated, despite the presence of organic signatures in the NIR region for some of these properties [1–6].

Ben-Dor (2002) has investigated and reported the several chromophores present in the soil matrix that might influence the VIS and NIR reflectance measurements of soils in the wavelength range between 400 and 2500 nm [30]. These chromophores were primarily related with clay minerals, carbonates, OM, water, iron oxides, and salts present in the soil matrix [30].

The identification and assignation of NIR bands for the measurements of these chromophores by different authors are provided in the following paragraphs. For example, one distinctive feature of smectite is its strong absorption band at approximately 1900 nm, associated with the combination of stretching and bending vibrations of structural water [30]. Bands at wavelengths 1412 nm and 2200 nm might be associated with the overtones of structural OH-stretching mode and water bound to surface oxygen of tetrahedral sheets [14,30]. Other authors reported that wavelengths around 1460 nm might be associated with water molecules involved in strong hydrogen bonding with clay surfaces [31]. In particular, this water absorption band can also be observed in the NIR spectrum of kaolinite, and overlaps with those exhibited by molecules such as AlFeOH at 2240 nm [31,32]. These authors also reported that the presence of AlOH groups might determine the increase absorbance around 2160 nm associated with the combination of OH stretching and deformation tones [31].

Other authors reported that the intensity of reflectance was reduced with the addition of OM into the soil matrix, where absorbances at 1440 nm (CH<sub>3</sub>), 1900 nm (OH combination) and 2240 nm (OH stretching and CH bending) were strongly accentuated [33,34]. The short wavelength range between 700 nm and 800 nm was reported to be correlated with the prediction of SOC particularly the indirect association with pigments derived from the decomposition of humic substances, chlorophyll, and phenolic compounds in this region [33,34]. Additionally, in this range, the third

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