Mid Infrared Spectroscopy for Rapid and Cheap Analysis of Soils

R.H. Merry and L.J. Janik

CSIRO Land and Water, Urrbrae, South Australia.

ABSTRACT

Due to advances in spectrometer hardware, computing and statistical software, mid infrared reflectance (MIR) spectra of soil samples have potential for fast, accurate and cheap soil analysis with particular application in the field and where high spatial density is needed. After minimal sample preparation, the MIR spectrum of a soil takes about two minutes to acquire and analyse. Recently, field portable spectrometers have become available and we have demonstrated that the technology can provide good quality prediction of soil properties, eg, carbonate and organic carbon, total nitrogen, cation exchange capacity and some exchangeable cations, electrical conductivity, pH, soil texture and a number of other properties, some of which are expensive to measure by conventional methods and not usually available. MIR analysis of soils is seen as a technology for the future, with applications that augment conventional soil testing and decision support, and capable of measurement in the field.

KEY WORDS

Soil analysis, mid infrared reflectance spectroscopy, MIR.

INTRODUCTION

Recent estimates suggest that more than 200,000 soil samples are analysed commercially in Australia each year, almost double the estimate made by Peverill (1) in the early 1990s. The majority of these conventional, laboratory-based analyses relate to soil pH, salinity, extractable phosphorus and nitrate nitrogen, exchangeable cations, organic carbon and extractable trace elements. These analyses are convenient in the laboratory because they are simple or highly automated, and are often well calibrated with field responses. However, there are other important soil properties that should be measured, but are not, because of great expense or poor understanding of their usefulness. In addition, the majority of soil samples are taken from surface soil layers and are assumed to be a “representative” sample of the whole paddock. As pointed out by Bramley and Cook (2), this common practice (unstratified sampling) frequently fails to properly account for soil variability within a paddock or to optimise subsequent fertiliser application or management. It also rarely takes account of subsoil constraints. There is a strong cost disincentive to collecting multiple surface soil or subsoil samples for routine testing.

The question arises as to what techniques may be available that could supply cheap and rapid soil analysis in agricultural systems and help optimise their management. Several are possible, such as remotely sensed properties using infrared or airborne radiometrics, but most have poor accuracy at the paddock scale or are limited by masking due to atmospheric dust and water, or by plant cover, and few are capable of sensing subsoil condition. The purpose of this paper is to discuss the potential of a new technology for soil sample analysis - diffuse reflectance mid infrared (MIR or DRIFTS) Fourier transform spectroscopy – and its application to agriculture.

RESULTS and DISCUSSION

What MIR can measure

As mentioned above, standard soil testing utilises a range of soil extractions that are important in assessing the adequacy or otherwise of plant nutrients, or used as indicators of important soil conditions that affect their management. Soil pH and organic carbon content are examples of the latter. Other indicators of soil condition such as particle size distribution, moisture storage capacity and clay mineral type are rarely analysed except in research projects, mainly due to their great expense. Soil carbon is likely to be increasingly important for Greenhouse Gas management. Soil carbon exists in several recognised “pools”, one of which is inert charcoal. Some soil carbon can be as much as 50% charcoal, but these pools are not distinguished by standard laboratory organic carbon analyses and soil charcoal, in particular, can only be measured using the ^{13}C-NMR spectroscopy costing about $500 per analysis. MIR is capable of predicting all of these above-mentioned properties, *simultaneously from a single spectrum*.

Table 1 shows a range of soil properties that MIR is capable of predicting in soils together with indicative coefficients of determination (R^2). Values of R^2 close to 1 indicate that MIR is almost as good as the laboratory technique against which it is calibrated. Within a paddock, or within uniform soil types, higher R^2 values are possible, for example, 0.99 for % $CaCO_3$ at Roseworthy and 0.90 for bulk density of Darling Downs clay soils. Many of the properties predicted from MIR spectra are those that generally change only slowly in soils so that, once analysed, re-analysis for that property may not be required, or only after a long time interval. Therefore, MIR spectral analyses are ideally suited for resource inventory.

Table 1. Soil chemical, physical and mineralogical properties, with indicative coefficients of determination (R^2) or capability predicted using MIR.

Soil property	*R^2*	*Characteristic*	*R^2*
Laboratory lime requirement	0.85	Clay mineralogy	yes
pH_{ca}	0.88	Elemental analysis (XRF) - SiO_2	0.97
0.01M $CaCl_2$ Al	0.69	Al_2O_3	0.92
0.01M $CaCl_2$ Mn	0.46	Fe_2O_3	0.93
Exchangeable Ca	0.89	MgO	0.80
Exchangeable Mg	0.88	P_2O_5	0.60
Exchangeable K	0.73	Particle size - % sand	0.93
Exchangeable Na	0.80	% silt	0.87
Exchangeable sodium % (ESP)	0.90	% clay	0.86
Sum exchangeable cations	0.93	Bulk density	0.62
$CaCO_3$ %	0.95	Volumetric moisture % @ -10kPa	0.67
Total organic C %	0.94	Volumetric moisture % @ 15 bar	0.81

OM fractions, charcoal	yes	Drained upper limit (Darling Downs)	0.93
Total N %	0.88	Water stable aggregates	0.67

How is it possible?

Over the past few years, computers have advanced greatly in speed and capability to manage large data sets, and to carry out complex calculations. MIR spectrometer design and the statistical software used to analyse spectra have also advanced. Partial least squares statistics have been used in the development of this technology. Advances in miniaturisation of MIR spectrometer hardware and improved stability have resulted in spectrometers small enough to be easily transported into the field. The combination of these developments has enabled new applications that can be applied to the rapid and simultaneous prediction of soil properties from infrared spectra.

Spectra are obtained from the mid infrared wavelength band from about 2.5 to 25 µm, where specific molecular vibrations are sensed and are strongly associated with functional groups common in soil mineral and organic matter.

MIR vs NIR

Near infrared reflectance (NIR) spectroscopy, which is a similar approach but uses a shorter wavelength band than MIR, has been used for analysis of minerals, forages, plant material and grains as well as for some soil materials, and has been reported, for example, by Dalal and Henry (3). We have compared MIR with NIR spectroscopy for prediction of soil properties and found MIR superior for several reasons, although NIR has been shown to be very useful. Technically, NIR relies on part of the spectrum that contains weak overtone and combination spectral frequencies that can be observed better as intense, fundamental vibrations in the MIR range. NIR is insensitive to quartz, a major component of most soils. However, NIR is well supported commercially, is well suited to field portability, remote sensing, copes better with moist samples and can deal with larger bulk soil samples because of its more intense sources and sensitive detectors.

Applications

Many potential and actual applications for MIR analysis are possible in either commercial soil testing or research. These include: soil analysis, decision support, soil property classification, soil survey and mapping, precision agriculture, diagnosis of soil problems, resource accounting, contaminated site characterisation and management, input data for models and as a replacement for pedotransfer functions. Of particular importance are situations that are data poor and cost constraints limit the amount of laboratory analysis that can be afforded but where MIR analysis can provide low cost, rapid prediction of properties or indicator level analyses. We have taken a portable MIR spectrometer to agricultural field days in Victoria and South Australia and been able to provide on-site analysis of soils from pits or samples provided by farmers. Existing “portable” MIR is actually “tethered” to a notebook computer and requires a power generator or DC battery source. Nevertheless, they can be operated from a vehicle, shearing shed or kitchen table.

Advantages of MIR

Several important advantages of MIR analysis have been mentioned above, but there are more. MIR spectra (from 30 to 50 scans) are acquired in less than one minute and simultaneous prediction of soil properties takes only a few seconds more. Alternatively, spectra can be acquired in batches and bulk predictions made for each particular property. We have achieved throughput in excess of 200 samples in 7 hours using a laboratory or field portable system that, with automation, could be substantially improved.

Samples used for MIR analysis require minimal treatment and only a few grams of powdered, air-dry soil are required. Better analyses can be obtained if samples are ground to less than about 0.1 mm particle size, but re-designed systems may avoid this and its associated costs. The use of a dry soil sample has advantages in that expensive or toxic chemicals are not required, there are no waste products and artificial solutions used in some extractions are avoided. Soil samples need to be air dry, or in a near dry, standard state, but this is normal for soil samples in conventional analysis.

Simultaneous analyses for more than twenty soil properties means that per analysis costs are low, with fast turn around times and digital output that can be directly applied using decision support software or as input to models. The quality of the analyses that are possible can only be as good as the quality of the data used for calibration and varies from near laboratory standard to indicator, “high, medium or low”. The technique can also be used for classification or quality control purposes. Additional discussion of some of these features can be found in Janik *et al*. (4).

Drawbacks

MIR technology has difficulty and performs poorly with the commonly used soil analyses that are based on the soil solution rather than the soil matrix, such as extractable P, S and N, due to their generally low concentration in the soil environment. However, MIR can predict total soil N, surface adsorption properties and many other total element concentrations in soils.

MIR analysis relies on calibration against recognised laboratory procedures for both chemical and physical properties. Therefore it can only be as good as the data against which it is calibrated. For many properties that MIR has capability to predict, there is often a paucity of high quality data and samples for calibration and, for many, there may in fact be high errors associated with the calibration sample.

CONCLUSIONS

We have been able to demonstrate new technology for soil analysis that has promise for application in agriculture and in soil research. MIR analysis is potentially much cheaper and faster than conventional soil testing, and a single spectrum can provide, simultaneously, useful information for more than 20 soil physical, chemical and mineralogical properties. It is likely that other soil properties, including some soil biology, could also be predicted if suitable calibration data and associated soil materials are available.

We have demonstrated rapid soil analysis in the laboratory and the field, and many areas of possible application of the technology. It is ideal for linking to decision support or modelling in soil management and resource inventory. Archiving of spectra is easy for future analysis using new calibrations – store the spectrum, not the soil sample. It has also been applied to achieve detailed and cheap analysis of soils from plots in field trials. Improvements to MIR technology for soil analysis could involve re-design of the IR source and reflectance sensing systems and the use of automation.

The future, outside research establishments, lies in adapting for effective commercial operation and its acceptance by clients as a technology for the provision of less expensive, but relevant, soil data for better land management.

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