

Application of FTIR Spectroscopy to Agricultural Soils Analysis

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1. Introduction

Soil is a very complex medium that contains minerals, organic matter, micro-organisms, air and water. Soil is one of the most important factors for agriculture and some soils are deemed more fertile than others. Soil fertility is directly related to factors such as nutrients concentrations or availability, organic matter content, acidity, moisture, etc., as well as to agricultural practice such as till vs. no-till (Desbiez et al. 2004) (Sá et al. 2009). Ensuring soil fertility is a basic requirement for any form of sustainable agriculture, yet in practice this seemingly trivial goal is very difficult to achieve due not only to the complexity of the soil medium itself, but also due to the complexity of the soil-crop-air interactions and to the fact that some processes require years before having any visible impact. Various recent studies have shown that soil fertility is declining in many farmlands due mainly either to inadequate farming practices (Gobeille et al. 2006), insufficient fertilization, in which case the soil reserves are depleted, or over-fertilization that results in pollution to the groundwater or toxic accumulation of chemicals in the soil. Avoiding such under- or over-fertilization is the chief goal of the so-called *precision fertilization* concept, which aims at delivering exactly the amount of nutrients required to sustain optimal growth of the crop. One of the main obstacles to the application of the precision fertilization concept, or the more general *precision farming* concept, is soil heterogeneity. Hence, although it is technically possible to perform a wide range of analyses and derive a soil fertility or health index such as the one proposed by Idowu et al. (2008), most of the required analyses are time-consuming, which in practice makes it impossible to map the soil properties of a field with the required spatial and/or temporal resolution. The need for fast and cheap methods that would enable the analysis of a large number of samples has been stressed in numerous studies (Viscarra Rossel&McBratney 1998b) and infrared spectroscopy has long been recognized as one of the most promising techniques (e.g. McCarty&Reeves 2006; Mouazen et al. 2007; Cécillon et al. 2009). As in other applications, the initial works were conducted mainly in the near-infrared (NIR) range for which instruments were readily available. Technological achievements in the mid-infrared (mid-IR) range during the last decade have made this spectral range much more attractive and an increasing number of soil studies are conducted using this spectral range. Although there is no doubt that near-infrared spectroscopy can be very useful for some analyses, several comparative studies have shown

the superiority of the mid-infrared techniques in most cases (McCarty&Reeves 2006; McCarty et al. 2002; Viscarra Rossel et al. 2006; Canasveras et al. 2010) and therefore the present chapter will focus solely on mid-IR techniques.

2. Mid-Infrared techniques commonly used for soil analysis

Infrared (IR) spectroscopy is based on the interaction of molecules with electromagnetic energy in the infrared spectral region, which is in the wavelength range of 0.8-1000 μm . This IR range is commonly divided into four regions, labeled near-, mid-, thermal- and far-infrared, respectively (Figure 1). The particularity of the mid-infrared range is that it includes the so-called fundamental vibrations of the molecules. When a molecule absorbs IR radiation at frequencies matching that of its own molecular vibrations, it results in an increase of the amplitude of the vibrations at these frequencies. Since each frequency corresponds to a given amount of energy and a specific molecular motion (e.g. stretching, bending or contracting of chemical bonds), the mid-IR spectrum can reveal the kind of molecular motions and bonds (functional groups) that are present in the molecule and hence can serve as a unique fingerprint of a specific compound. Furthermore, most functional groups have characteristic IR absorption bands that do not change much from one compound to another. By comparison, the near-infrared range is dominated by overtones and combinations of these fundamental vibrations, which makes the interpretation of the NIR spectra much more difficult.

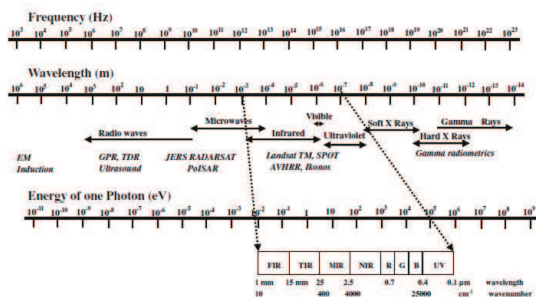


Fig. 1. The electromagnetic spectrum with emphasis on the ultra-violet - infrared range. Reproduced from Viscarra Rossel et al. (2006).

Nowadays, Fourier Transform Infrared (FTIR) is the preferred method for mid-IR spectroscopy as it provides quantitative information in a rapid and accurate fashion. A typical FTIR spectrometer obtains an infrared spectrum by collecting the interferogram of a sample signal, which contains all the infrared frequencies, applies the Fourier transform to the digitized signal, and outputs the spectrum. Such a FTIR spectrometer relies on an interferometer, which splits to radiation beam into two beams that are recombined after a path difference has been introduced (Griffiths&de Haseth 1986). The most common interferometer is the so-called Michelson interferometer, which consists of a beam splitter located between two perpendicular mirrors, one of which can move along an axis perpendicular to its plane (Figure 2). At the beam splitter, the radiation beam from the infrared source is partially reflected to the fixed mirror and partially transmitted to the moveable mirror. The moveable mirror is moved in a highly controlled fashion to create the

path difference between the two beams. After the beams return to the beam splitter, they interfere and are again partially transmitted and partially reflected to the detector. Due to the effect of the interference, the intensity of each beam passing to the detector and returning to the source depends on the path-length difference between the two beams. The two beams can undergo constructive interference, destructive interference or a combination of both, depending on the path-length difference. Constructive interference, which yields a maximum detector signal, occurs when the optical path difference is an integer multiple of the wavelength. The variation in the energy that reaches the detector as a function of the path difference yields the interferogram, which is the integral of all interference patterns produced by each wavelength. The detected interferogram can not be interpreted directly, but has to be "decoded" using the well-known Fourier Transformation (Griffiths&de Haseth 1986). Fourier transform is typically thought of as decomposing a signal into its component frequencies and their amplitudes. The Fourier transform is an integral transform that re-expresses a function in terms of sinusoidal basis functions, i.e. as a sum or integral of sinusoidal functions multiplied by some coefficients ("amplitudes"). The general idea is that a multiplication of the input waveform of unknown amplitude and frequency (interferogram signals) by a known reference frequency of unity amplitude (the analyzing wave) can give us the unknown amplitude and original frequency. Thus, by using a frequency-adjustable analyzing wave, each digitized point of the interferogram can be transformed from the time (or optical retardation) domain to the frequency domain, which results in the IR spectrum. When a single interferogram is thus Fourier-transformed, a so-called single-beam spectrum is generated, which is the raw detector response versus the wavelength. In order to produce the absorption spectrum of a sample, the sample single-beam spectrum must be normalized against a background spectrum taken with no sample in the beam path. The absorption spectrum can be presented equivalently as a transmittance ($T = I/I_0$) or absorbance ($A = \log_{10} I_0/I$) spectrum, where I is the intensity measured with the sample in the beam and I_0 is the intensity measured from the background spectrum.

Direct transmittance is the oldest and most straightforward spectroscopic technique, which is based on the absorption of the IR radiation as it passes through the sample. Clearly, this technique is applicable only to samples that do not absorb all the incoming IR energy and are sufficiently transparent in this spectral range. For highly absorbent samples, such as soils, it is necessary to prepare a pellet that embeds the soil sample in a transparent matrix, most usually KBr. The pellet preparation involves grounding 2-3 mg of soil with ~1 g of KBr using a mortar and pestle and using a hydraulic press and die to create a thin, IR-transparent disk. The main advantage of this technique is that it yields very clear and information-rich signals. Its main disadvantages are the lengthy preparation required to prepare the pellets and the fact that it is difficult to obtain quantitative results. Also, since only a few mg of soils are used for the preparation of each pellet, the resulting spectrum may not be representative of the bulk soil. For these reasons, transmittance measurements are rather rarely used in soil analysis and the reflectance and photoacoustic methods described below are preferred.

2.1 Diffuse reflectance

Nguyen et al. (1991) pointed out to two main drawbacks of the transmittance technique in addition to the time-consuming sample preparation: (1) possible reaction of the sample with the halide matrix, and (2) scattering and/or total absorption for samples with high concentrations and large particles relative to the infrared wavelengths. To circumvent these limitations, Nguyen et al. (1991) introduced the use of diffuse reflectance (DRIFT) for soil

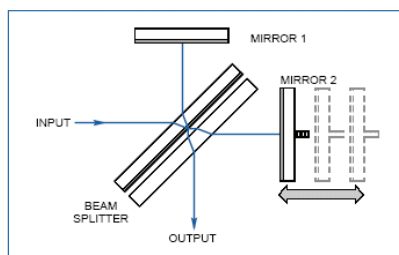


Fig. 2. Schematic description of a Michelson interferogram.

analysis. While the study of Nguyen et al. (1991) was purely qualitative and restricted to band assignments, the subsequent articles of Janik et al. (1995) and Janik&Skjemstad (1995) showed that mid-IR DRIFT could be used to quantify various soil components. Since then, the use of mid-IR DRIFT has been investigated in numerous soil studies (see excellent review paper of Reeves III 2010), and it is arguably the mid-IR spectroscopic method most commonly used for soil analysis. DRIFT spectroscopy is mainly concerned with radiation emerging from a non-mirror or matt surface after it has undergone absorption, refraction, reflection and scattering in the bulk material. DRIFT spectra are subject to nonlinear scaling of the intensity which reduces the intensity of strongly absorbing bands in comparison to weaker bands. Thus, low intensity bands appear to be enhanced in DRIFT spectra. The specular component becomes increasingly significant at high sample concentrations and for large particles, and the occurrence of strong specular reflection explains for instance why the presence of inorganic carbon interferes with the development of calibrations for soil organic carbon (Reeves et al. 2005). In order to avoid such non-linearities and spectral distortions, the use of samples diluted with KBr has long been advocated and such KBr dilution is still used in many studies. However, using KBr-diluted samples increases the sample preparation time and may cause interferences due to ion exchange between the sample and the KBr matrix or adsorption of water onto the KBr (Bertrand et al. 2002). Janik&Skjemstad (1995), Janik et al. (1998) and Reeves et al. (2001) have shown that quantitative analysis can also be performed on mid-IR spectra of neat (undiluted) soil samples. These findings were further supported by the comparative study of Bertrand et al. (2002) who compared results obtained using neat and KBr-diluted samples and concluded that KBr dilution does not improve the accuracy of the measurements.

2.2 Attenuated total reflectance

In the Attenuated Total Reflectance (ATR) method, the IR radiation propagates through a crystal with a high refractive index that is in contact with the sample (Figure 3). Mirrors are used to direct the IR beam toward the crystal at an angle that exceeds the critical angle for internal reflection, so that the radiation undergoes multiple reflections within the crystal.

This critical angle θ_c depends on the refractive indices of the sample and ATR crystal according to

$$\theta_c = \sin^{-1}\left(\frac{n_2}{n_1}\right) \quad (1)$$

where n_1 and n_2 are the refractive indices of the crystal and the sample, respectively. Due to the quantum mechanic properties of the light, the electromagnetic field extends beyond the

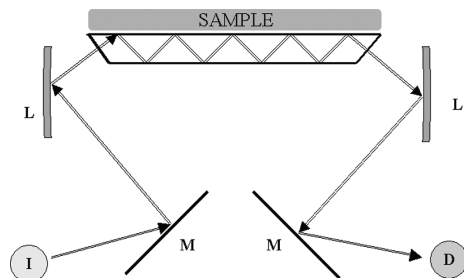


Fig. 3. Attenuated total reflectance (ATR) configuration. I denotes the incoming light (from the interferometer), D denotes the detector, L and M are lenses and mirrors. Reproduced from (Etzion et al. 2004)

crystal surface for a short distance known as the *evanescent field*. If a sample is applied directly onto the surface of the ATR crystal, some of the IR radiation (i.e., the evanescent wave) is absorbed by this sample, so that the sample absorbance spectrum can be obtained. The evanescent wave decays exponentially with the distance from the surface of the crystal. The depth of penetration of the evanescent wave d_p is defined as the distance from the crystal-sample interface at which the intensity of the evanescent wave decays to 37% ($1/e$) of its original value, and is given by

$$d_p = \frac{\lambda}{2\pi n_1 \sqrt{\sin^2 \theta - (n_2/n_1)^2}} \quad (2)$$

where λ is the radiation wavelength. The penetration depth and the total number of reflections along the crystal can be controlled to some extent either by varying the angle of incidence of the radiation (θ) or through the selection of the crystal material. The penetration depth is typically less than $10 \mu\text{m}$, so that very good contact between the sample and the crystal is critical in order to obtain reliable and reproducible results.

The first use of ATR for soil analysis was reported by Ehsani et al. (2001), who attempted to determine nitrate concentration using ATR spectra of dry soil samples. This study demonstrated the difficulty of obtaining adequate contact between the soil and the ATR crystal, but also showed how the results could be greatly improved by using a soil paste or slurry. Such a technique was further developed by Shaviv et al. (2003), Linker et al. (2004), Linker et al. (2005) and Borenstein et al. (2006) who used samples consisting of soil pastes close to water saturation. Since nitrate is highly soluble in water and is not fixed in the soil matrix, all the nitrate is present in the liquid phase of the soil paste, which has several advantages. First, since the paste moisture content is less than $1 \text{ g } [\text{H}_2\text{O}]/\text{g } [\text{soil}]$, the nitrate concentration in the liquid phase is higher than in the dry soil. Second, much better contact is obtained between the ATR crystal and the liquid phase than could be obtained between the ATR crystal and the dry soil. Finally, the original moisture of the soil sample has no influence on the measurement. However, water exhibits very strong absorbance bands in the mid-IR range, which may distort or hide bands of interest. This is illustrated in Figure 4 which shows the spectra of de-ionized water, de-ionized water with $1000 \text{ mg}[\text{N}]/\text{kg}[\text{water}]$ nitrate, and a paste of sandy soil with $870 \text{ mg}[\text{N}]/\text{kg}[\text{water}]$ nitrate. Distortion and shift of

the spectra can be observed, especially in the regions indicated by circles. The magnitudes of these changes are comparable with the size of the nitrate signal and would cause significant inaccuracies if straightforward estimation of nitrate was performed. Therefore an accurate water subtraction procedure such as the one developed by Linker et al. (2004, 2005) should be applied to the spectra prior to the quantitative analysis.

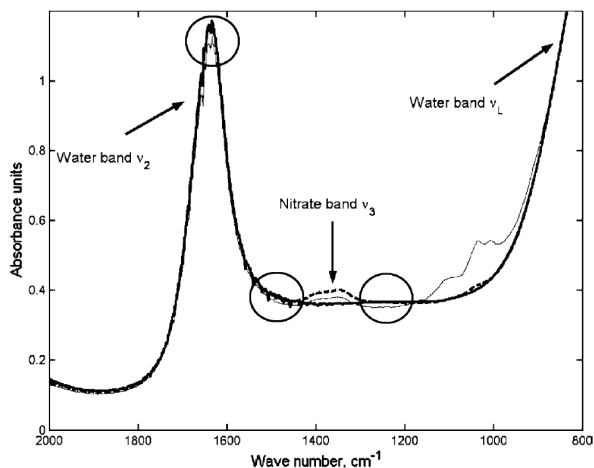


Fig. 4. Spectra of de-ionized water, de-ionized water with 1000 mg[N]/kg[water] nitrate, and a paste of sandy soil with 870 mg[N]/kg[water] nitrate. The circles indicates the regions in which shifts and distortions of the spectra are most clearly visible. Reproduced from Linker et al. (2005).

2.3 Photoacoustic spectroscopy

Fourier transform infrared photoacoustic spectroscopy (FTIR-PAS) differs from the previous methods in the sense that it relies on complete absorption of the incoming radiation by the sample. The sample is placed in a sealed enclosure that is purged with He to avoid atmospheric interferences and to which is connected a highly sensitive microphone which records the pressure waves that result from the local heating induced by the absorbed radiation (McClelland et al. 2002) (Figure 5). The recorded spectrum depends on the absorption properties of the sample, its thermal diffusivity, and the thermal penetration depth. Therefore, photoacoustic spectra are more difficult to interpret than reflectance ones and there is no one-to-one correspondence between the spectra obtained with both techniques. Also, photoacoustic spectra are much more prone to measurement noise. Nonetheless, since this method can be used with highly absorbing samples without any pretreatment, it is well suited for soil samples analyses and its use has been reported in several recent studies (Du et al. 2008a, 2008b, 2009b).

3. Data processing

Due to the large amount of data generated by FTIR spectrometers and the complexity of the spectra, it is imperative to use chemometrics procedures to analyze the data. A detailed

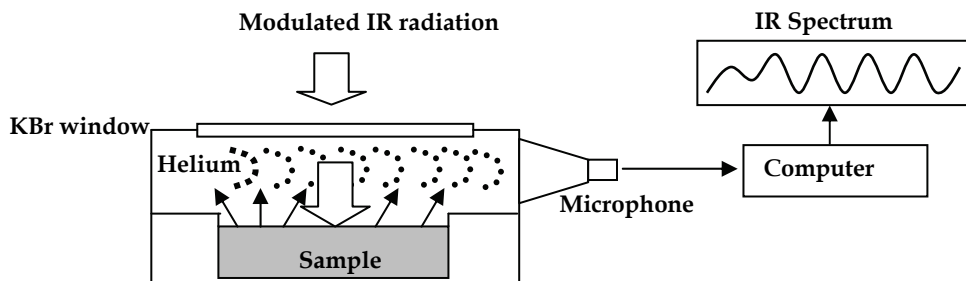


Fig. 5. Schematic description of FTIR photoacoustic spectroscopy. Reproduced from Du et al. (2008a).

description of such procedures can be found in various textbooks such as Brereton (2003) or Chau et al. (2004). Partial Least Squares (Wold et al. 2001) is the procedure most commonly used for quantitative determination of one or several soil components (see for instance the excellent compilation table in Viscarra Rossel et al. (2006)). PLS is an easy-to-use straightforward procedure that is available in standard statistical and chemometrics softwares, which probably explains its popularity. The main limitation of PLS is that it assumes linearity of the data, but the good results reported in most soil studies show that this does not appear to be too restrictive an assumption when analyzing soil spectra. Exceptions to this generally linear behavior were reported for instance by Janik&Skjemstad (1995) and Janik et al. (2009), especially at very high concentrations. However, Janik et al. (2009) reported that in those cases where PLS was not capable of providing a good prediction model, adding a non-linear element in the form of a neural network did not improve the results significantly.

The *a priori* assumption of linearity can be avoided altogether by using procedures such as wavelet decomposition and neural networks. An example of such a procedure is depicted in Figure 6. In this procedure, wavelet decomposition is used to compress the data and obtain a low-dimensional representation of the spectra. Although wavelet decomposition by itself does not produce a compressed representation of the original data, data reduction can be achieved by eliminating the wavelet coefficients that do not contain valuable information. Various approaches have been reported in the literature for selecting the most relevant coefficients, such as eliminating all "small" coefficients using for instance either thresholding (Kai-man Leung et al. 1998; Ehrentreich 2002), entropy (Kai-man Leung et al. 1998), mutual information (Alsberg et al. 1998), maximum likelihood (Leger&Wentzell 2004), or genetic algorithms (Depczynski et al. 1999), or retaining only the coefficients with the highest variance (Trygg&Wold 1998) as depicted in Figure 6. Once data compression has been achieved, the remaining coefficients can be used as input variables for a neural network that creates a non-linear mapping between these inputs and the property (or properties) of interest. The neural network can also be replaced by a simpler linear regression as in Viscarra Rossel&Lark (2009), in which case a hybrid model that contains both linear and non-linear stages is obtained.

Since the wavelet transform decomposes the signal into components at different scales (or loosely speaking, components of different widths), it is a very powerful tool for resolving overlapping bands and separate the bands of interest from the background and interferences. For instance, Jahn et al. (2006) used such an approach to distinguish between the strongly-overlapping absorbance bands of nitrate and calcium carbonate in the ATR spectra of calcareous soils (Figure 7).

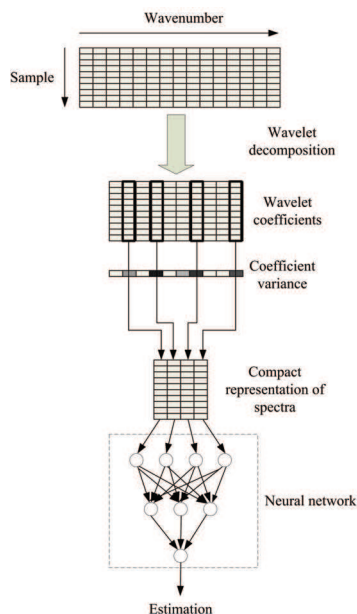


Fig. 6. Schematic representation of a prediction model combining wavelet decomposition of the spectra and a neural network

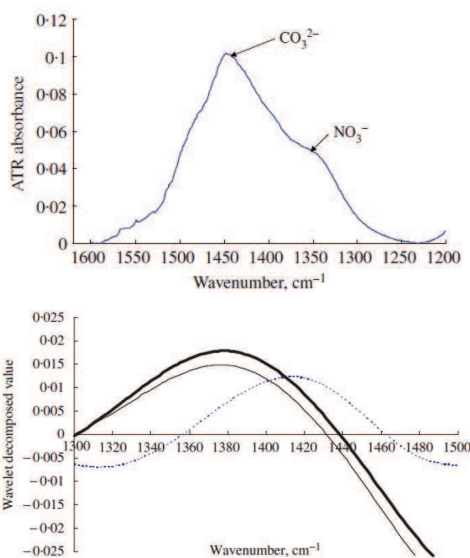


Fig. 7. Overlapping bands of nitrate and carbonate in ATR spectra of calcareous soils (Top frame) and the wavelet decomposed values at scale 2 (dashed, attributed to carbonate) and at scale 3 (attributed to nitrate, 14 ppm and 120 ppm N-NO₃) (Bottom frame). Reproduced from Jahn et al. (2006).

4. Most common applications

4.1 Estimation of soil nutrients and organic matter

Soil nutrients, such as C, N, P, K, S, Ca and microelements, play a primordial role in the development of agricultural crops and hence determination of their concentrations is crucial to the application of the precision agriculture concept. Viscarra Rossel et al. (2006) compiled an excellent review of the studies dedicated to the estimation of these parameters using diffuse reflectance. Table 1 present a non-exhaustive list of studies that focused on the determination of carbon, total nitrogen, nitrate, potassium, phosphorus and organic matter using diffuse reflectance, ATR and photoacoustic spectroscopy. Table 1 clearly shows that carbon, and in particular organic C, is the property most commonly determined, using DRIFT. Most studies reported very good results with correlation coefficients (R^2) between the actual and estimated values higher than 0.90. A noticeably much poorer result was reported by Reeves&Smith (2009) ($R^2=0.60$). This latter study was not restricted to agricultural soils as the previous studies (some of which included a number of samples similar to that of Reeves&Smith (2009)), but included soil samples from national forests, rangelands, woodlots, etc. and Reeves&Smith (2009) hypothesized that this wide range of soil uses was responsible for the poor performance of the regression models. Acceptable results were also reported for estimation of total nitrogen ($R^2>0.80$), using either DRIFT or photoacoustic spectroscopy. For nitrate, Viscarra Rossel et al. (2006) did not find any correlation between DRIFT spectra and nitrate concentration. This finding contrasts sharply with the good results that can be obtained using the ATR technique, for which the typical determination errors range from 5 to 25 mg[N]/kg[dry soil] for realistic agricultural field concentrations. The largest determination errors correspond to calcareous soils for which nitrate determination is hindered by the absorbance band of carbonate that overlaps the nitrate band (Linker et al. 2004, 2005, 2006; Borenstein et al. 2006; Jahn et al. 2006). For potassium, phosphorous and organic matter conflicting findings have been reported. Bertrand et al. (2002) reported that DRIFT could be used to estimate potassium concentration ($R^2=0.85$). Acceptable results were also reported by Du et al. (2009b) who used photoacoustic spectroscopy ($R^2=0.79$). McCarty&Reeves (2006) and Reeves&Smith (2009) obtained relatively poor but still potentially useful results using DRIFT (R^2 of 0.60 and 0.76, respectively), but Viscarra Rossel et al. (2006) concluded that DRIFT spectroscopy was not suitable for estimating potassium concentration ($R^2=0.40$). For phosphorous, Janik et al. (2009) and Du et al. (2009b) reported R^2 values of 0.87 and 0.81 using DRIFT and photoacoustic spectroscopy, respectively. However, Bertrand et al. (2002), McCarty&Reeves (2006) and Viscarra Rossel et al. (2006) did not find a relationship between DRIFT spectra and phosphorous ($R^2<0.40$). For organic matter, very good results were obtained using photoacoustic spectroscopy (Du et al. 2007, 2009b) and DRIFT (Masserschmidt et al. 1999), with R^2 values above 0.90 in all three studies. However, very poor correlation between DRIFT spectra and organic matter content was reported by Canasveras et al. (2010).

The somewhat conflicting results reported in some of the DRIFT studies emphasize the need for standardization of the analyses (both analytical reference analyses and DRIFT spectroscopy) and underscore the problem of transferability of the results (See Section 5.1). Photoacoustic spectroscopy appears to be a very promising technique which should certainly be investigated in further studies.

	Diffuse reflectance	Attenuated total reflectance	Photoacoustic
Organic C	Janik&Skjemstad (1995); Janik et al. (1998); McCarty et al. (2002); Reeves et al. (2002); Reeves (2009, 2010); Reeves&Smith (2009); McCarty&Reeves (2006); Viscarra Rossel et al. (2006, 2008); Viscarra Rossel&Lark (2009); Janik et al. (2009); Zimmermann et al. (2007); McBratney et al. (2006)		
Total C	McCarty et al. (2002); Reeves et al. (2001, 2002); Reeves (2009, 2010); Viscarra Rossel et al. (2008); Minasny et al. (2009); Reeves&Smith (2009)		
Total N	Janik&Skjemstad (1995); Reeves et al. (2001); McCarty&Reeves (2006); Viscarra Rossel et al. (2008)		Du et al. (2009b)
Nitrate	Viscarra Rossel et al. (2006); Verma&Deb (2007)	Ehsani et al. (2001); Shaviv et al. (2003); Linker (2004); Linker et al. (2004, 2005, 2006); Borenstein et al. (2006); Jahn et al. (2006);	
Potassium	Bertrand et al. (2002); McCarty&Reeves (2006); Viscarra Rossel et al. (2006); Minasny et al. (2009); Reeves&Smith (2009)		Du et al. (2009b)
Phosphorus	McCarty&Reeves (2006); Viscarra Rossel et al. (2006); Janik et al. (2009); Minasny et al. (2009)		Du et al. (2009b)
Organic matter	Masserschmidt (1999); Canasveras et al. (2010)		Du et al. (2007, 2009b)

Table 1. List of studies that used reflectance and photoacoustic spectroscopy for the estimation of soil carbon, total nitrogen, nitrate, potassium phosphorus and organic matter

4.2 Determination of soil moisture

Water in itself is essential for plant growth and its presence in the soil influences numerous properties such as the availability of oxygen and nutrients, microbial activity, swelling and shrinking of clays or soil stability. Since the methods traditionally used to estimate water-related soil properties are time consuming, much research has been devoted to the development of alternative methods. In particular, very good results have been reported for some of these properties using near-infrared spectroscopy under laboratory conditions (Mouazen et al. 2005, 2006; Viscarra Rossel&McBratney 1998a) and encouraging results have been reported for in-situ field measurements (Mouazen et al. 2005). A summary of the main results obtained with mid-IR DRIFT spectroscopy is presented in Table 2. With the exception of Dataset #1 in Tranter et al. (2008), mid-IR spectroscopy was capable of estimating to some extent water retention at -10kPa and -1500kPa, with R^2 values ranging from 0.64 to 0.81 and from 0.66 to 0.89, respectively. However, the study of Bertrand et al. (2002) clearly shows that KBr dilution of the samples or high CaCO_3 concentration deteriorate the results. Although this has not been specifically verified, the very poor results obtained by Tranter et al. (2008) on Dataset #1 were most probably due to the fact that the spectra were recorded from intact soil cores rather than from grounded samples as in all the other studies. Regarding moisture of air-dried and oven-dried soil, the few results available are very good, unless the soil has a high CaCO_3 concentration.

4.3 Soil characterization

The soil physical structure affects various physical, chemical and biological processes such as for instance water infiltration and retention or root penetration and proliferation. With this respect, clay is the component most often studied by mid-IR spectroscopy, although some studies also attempted to estimate sand or silt content (McBratney et al. 2006; Viscarra Rossel et al. 2008). For clay, R^2 values of 0.85 or more were reported by Janik&Skjemstad (1995), Viscarra Rossel et al. (2008) and Viscarra Rossel&Lark (2009). Reasonably good results were reported by Janik et al. (2009), Canasveras et al. (2010) and Janik et al. (2009), with R^2 value of 0.84 and 0.82, respectively, but lower R^2 values (0.74-0.79) were reported by Bertrand et al. (2002), McCarty&Reeves (2006), Minasny et al. (2009) and McBratney et al. (2006). No explanation has been offered to explain such a variability of the prediction performances. In addition to the previous DRIFT studies, Du et al. (2007) reported very good results ($R^2 > 0.90$) using photoacoustic spectroscopy and Du et al. (2008b) further showed that this method can be used to differentiate between different types of clays. Another important soil component that can be estimated by mid-infrared spectroscopy is carbonate. In this case the results are much more consistent, with R^2 values of 0.95 or more reported in the studies of Janik&Skjemstad (1995), Bertrand et al (2002), Canasveras et al. (2010) and Du et al. (2008b). Linker et al. (2006) and Du et al. (2008a) showed that the spectral information related to carbonate and other soil constituents can be used to discriminate between soils, and Linker et al. (2006) further showed that such a automatic discrimination can improve the estimation of nutrients such as nitrate.

5. Current challenges and emerging applications

5.1 Spectral libraries and model transferability

The results presented in the previous Section clearly demonstrated that mid-IR spectroscopy can be used to determine accurately a series of soil characteristics and properties under

Study	Water retention at -10kPa or 120cm	Water retention at -1500kPa	Moisture of air-dried soil	Moisture of oven-dried soil
Bertrand et al. (2002)	0.92‡		0.92	
	0.84‡ (KBr diluted samples)		0.86 (KBr diluted samples)	
	0.74‡ (CaCO ₃ >2%)		0.68 (CaCO ₃ >2%)	
McBratney et al. (2006)	0.64†	0.66†		
Janik et al. (2007)	0.79	0.84		
Tranter et al. (2008) (Dataset #1 - intact cores)	0.02	0.50		
	0.48†	0.71†		
Tranter et al. (2008) (Dataset #2 - crushed samples)	0.85	0.89		
Janik et al. (2009)	0.81	0.89		0.89

Table 2. R² values between the actual soil moisture or water retention and the one estimated from mid-IR spectra. The results were obtained using neat ground samples unless otherwise indicated. † indicates that results obtained indirectly using properties estimated by mid-IR spectroscopy and pedotransfer functions. ‡ indicates that the result correspond to water retention at 120cm water tension

laboratory conditions. However, two questions still remain mostly unanswered: (1) could a regression model developed by one group of researchers be readily applied by other researchers and (2) would it be possible to establish spectral libraries that combine spectra from different sources? Such issues are of course not restricted to mid-IR spectroscopy but are also relevant to NIR spectroscopy (Cécillon et al. 2009). These two issues are related since in the absence of such libraries each research team tends to work with spectra recorded “in-house” using experimental procedures that are, at least to some extent, specific to that specific laboratory. Furthermore, due to the extensive work required to collect soil samples and to perform detailed chemical analyzes of these samples, most studies are still based on soil samples belonging to a specific geographic area. The issue of mid-IR model transferability was recently addressed by Minasny et al. (2009) who concluded that “Due to the differences in the origins of the soil and in the laboratory measurement procedures, calibration functions from one region do not perform well on another one”. They further emphasized that in their opinion the cause for this lack of transferability lies mainly in the difference in laboratory techniques, different analytical procedures, and inter-laboratory

bias. The creation of a library of mid-IR DRIFT spectral of soils was considered by Viscarra Rossel et al. (2008) who emphasized three main prerequisite for the development of such a library: (1) it should describe adequately the soil variability in the region in which it is to be used, (2) experimental procedures, and in particular sample handling, preparation, storing and scanning must be standardized and (3) the analytical data used as reference should be acquired using reliable and accredited analytical procedures. This issue was also addressed by Reeves III in his recent review on the use of NIR and mid-IR DRIFT for soil analysis (Reeves III 2010) in which he emphasized that "Spectral libraries for quantitative analysis will be useless, or worse deceptive, if users base results on combining spectra from differing sets of samples that have not been standardized." However, as the study of Reeves&Smith (2009) clearly demonstrated, standardization in itself does not guarantee accurate results, even for properties that seem trivial to determine such as organic carbon. In this case, Reeves&Smith (2009) explained their poor results by the fact that their database included soils of various usages rather than to be restricted to agricultural soils. Finally, it must be noted that since specular reflection occurs for both organic and non-organic fractions of soil, libraries of spectra collected by other means than diffuse reflectance would be largely useless for comparing mineral spectra to soil spectra (Reeves et al. 2005). All these factors underline the complexity of the task at hand if one was to contemplate the creation of a truly universal soil spectral library.

5.2 Indirect estimation of additional soil properties

In addition to those properties that can be measured directly by mid-infrared spectroscopy, there is a large number of important soils properties that are not associated with distinct absorbance bands. In such cases McBratney et al. (2006) propose to use the estimates obtained by mid-IR spectroscopy in an inference system that uses pedotransfer functions. This approach is illustrated in Figure 8: Once regression models based on mid-IR spectra have been calibrated for properties such as clay, silt, sand and organic carbon, these models are used to estimate the same properties of a new sample, together with their respective uncertainties. These values are then used to predict the bulk density, the water content at field capacity and wilting point, and finally the available water capacity.

An important feature of this approach is that the determination errors are propagated through the various estimation stages so that a confidence interval can be associated with each prediction (Figure 9). Tranter et al. (2008) showed how such an approach improved considerably the estimation of soil water retention, which was very poorly estimated directly from the mid-IR spectra (See Table 2). Minasny&McBratney (2008) also reported more parsimonious models and greater accuracy when using an inference system then when using straightforward PLS regression on the mid-IR spectra. Such an approach may help solving the "model transferability" problem discussed in the previous section and further work should be devoted to validating and improving this interesting approach.

5.3 On-the-go sensing and combination with GIS

In order to achieve "precision farming", the information obtained from soil analyzes must be combined with a Geographic Information System (GIS) platform in order to create overlaying maps of soil characteristics, water content, nutrient availability, yield, etc. In addition to measurement accuracy, a key issue is the number of sampling points and the spatial resolution of the measurements. The development of "on-the-go" sensors is of

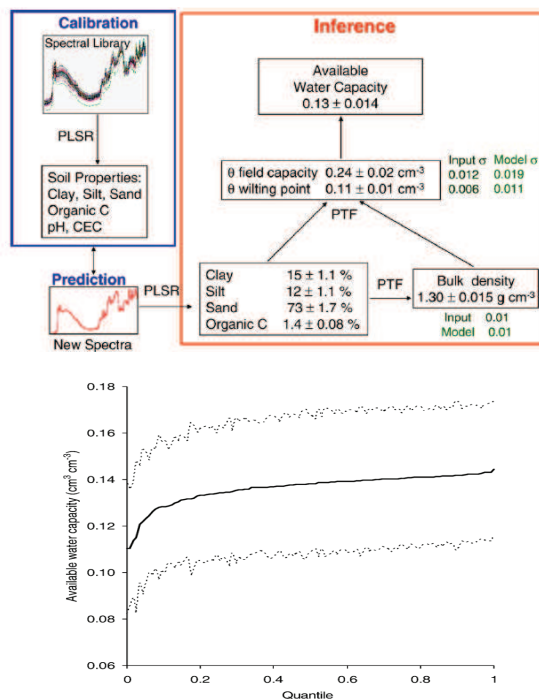


Fig. 8. Top frame: Schematic description of the combination of mid-IR spectroscopy and inference models as suggested by McBratney et al. (2006). Bottom frame: Quantiles of the available water capacity estimated according to the inference scheme. Reproduced from McBratney et al. (2006).

primordial importance (Viscarra Rossel & McBratney 1998b) and considerable research efforts have been devoted to the development of fast, fully automated and geo-referenced measurement systems (Sibley et al. 2009; Mouazen et al. 2007; Christy 2008; Adamchuk et al. 2004, 2005; Sinfield et al. 2010). Among the spectroscopy-based methods, the use of NIR has been investigated more actively, mostly due to the lower price and higher robustness of the equipment. Indeed, in their review paper Sinfield et al. (2010) concluded that the “the FT-IR ATR technique, while very accurate and fast, makes use of expensive and delicate equipment (e.g., moving mirror in interferometer) which is not readily amenable to an on-the-go setting” but that development of sensors based on a limited set of wavebands, as suggested by Linker (2004) and Jahn et al. (2006), could “enhance the potential to apply reflectance based approaches in the field by limiting the sophistication of requisite equipment”. At any rate, considerable improvements are still required before large-scale implementation could be considered.

5.4 Monitoring of N isotopes

Nitrogen, either naturally present in the soil or added as fertilizer, may undergo a series of complex transformations. These transformations are interdependent and depend on a large number of variables, so that isolating specific processes or pathways is very challenging. One of the methods used to study these processes consists of enriching the soil with stable

^{15}N isotopes and monitoring the concentration of ^{15}N in the by-products of the various reactions (Stevens et al. 1993; Stevens&Laughlin 1994; Baggs 2008). Such studies require the quantification of ^{14}N and ^{15}N , which is done by isotope ratio mass spectrometry (IRMS). However, expensive and laborious preparation of the samples is required to convert the N species into forms suitable for the IRMS measurements and the method can not realistically be used to analyze a large number of samples during an experiment. Du et al. (2009a) showed how mid-infrared spectroscopy could provide a much faster and cheaper alternative for N-isotope tracing, albeit with much lower accuracy than IRMS. The method is based on the observation that since the mid-infrared range corresponds to the fundamental vibrations of a molecule, which depend on the atoms' mass, the absorbance bands of ^{14}N -based and ^{15}N -based compounds are slightly shifted relative to each other, so that the concentration of each species can be estimated. This spectral shift between $^{14}\text{N}\text{-NO}_3$ and $^{15}\text{N}\text{-NO}_3$ is shown in Figure 9.

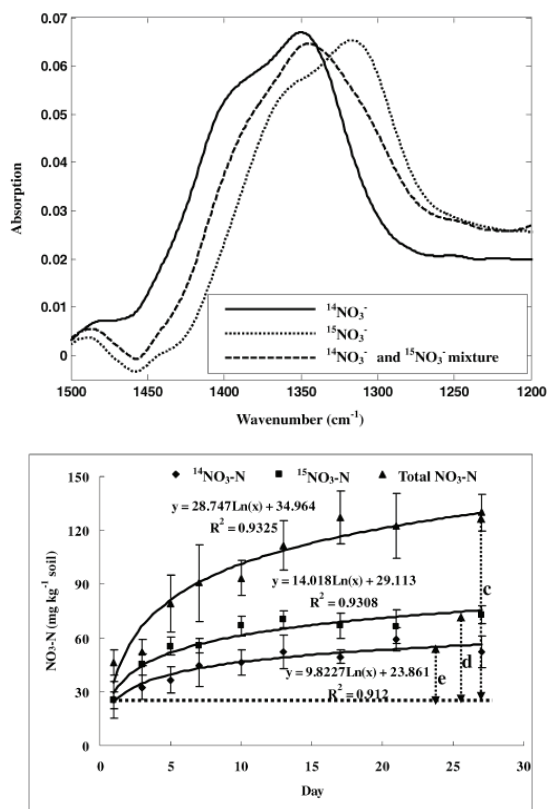


Fig. 9. Top frame: FTIR-ATR spectra of $^{14}\text{N}\text{-NO}_3$ and $^{15}\text{N}\text{-NO}_3$ in water. Bottom frame: Nitrate formation during an incubation experiment as estimated from FTIR-ATR measurements. Nine sub-samples were analyzed at each sampling point. "c" is the total amount of nitrate formed. "d" and "e" are the formed $^{15}\text{N}\text{-NO}_3$ and $^{14}\text{N}\text{-NO}_3$, respectively. Reproduced from Du et al. (2009a).

Using PLS regression models calibrated using saturated soil pastes spiked with $^{14}\text{N-NO}_3$ and $^{15}\text{N-NO}_3$, Du et al. (2009a) were able to estimate the $^{14}\text{N-NO}_3$ and $^{15}\text{N-NO}_3$ concentrations in a non-calcareous soil with determination errors of less than 6 mg[N]/kg[dry soil], which enabled them to monitor separately the formation of $^{14}\text{N-NO}_3$ and $^{15}\text{N-NO}_3$ during an incubation experiment (Figure 9). Although the measurement uncertainties reported in Figure 9 may seem rather large, the low cost and short time required for the FTIR-ATR measurements would make it possible to perform and average more measurements than as done in the study of Du et al. (2009a), and thus reduce the measurement uncertainties. After further validation of the approach with other soils, including with calcareous soils in which the carbonate absorbance band overlaps the nitrate absorbance band and interferes with nitrate determination (Linker et al. 2004, 2005, 2006), and extension of the method to monitoring soil NH_4 and/or NO_2 species, this method would provide a very powerful and cheap tool for studying soil nitrogen transformations.

6. Conclusion

The abundant studies conducted in the mid-IR range have demonstrated the potential that this technique holds for rapid and inexpensive soil analysis. A major advantage of spectroscopy techniques in general and mid-IR in particular is that several properties can be determined from a single spectrum, which greatly reduces the costs of analysis compared to conventional laboratory techniques. In addition, the measurement is very rapid so that a large number of samples can be easily screened or measurements could be conducted "on-the-go", at least in principle. However, several problems still need to be solved before this technology could be upgraded from the research laboratory into routine analyses. The most pressing issue appears to be the standardization of the FTIR and conventional procedures used to analyze the samples, which would make it possible to consider the establishment of spectral libraries similar to those existing in other FTIR fields. Such libraries would provide the basis necessary for developing robust chemometrics models, based either solely on mid-IR spectra or combining mid-IR spectra and pedotransfer functions, valid not only at the local but also at the regional scale.

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