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Assessment and monitoring of soil quality using near infrared reflectance spectroscopy (NIRS)

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– *Review paper* –

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Summary

Soil degradation processes have dramatically increased in their extent and intensity over the last decades. Progressively, actions have been taken in order to evaluate and reduce the major threats that have already wreaked havoc on soil conditions. Efficient and standardized monitoring of soil conditions is thus required but soil quality research is facing an important technological challenge because of the number of properties involved in soil quality. The objective of the present review is to examine critically the suitability of near infrared reflectance spectroscopy (NIRS) as a tool for soil quality assessment. We first detail the soil quality-related parameters (chemical, physical and biological) that can be predicted with NIRS through laboratory measurements. The ability of imaging NIRS (airborne or satellite) for mapping a minimum data set of soil quality is also discussed. Then we review the most recent research using soil reflectance spectra as an integrated measure of soil quality, from global site classification to the prediction of specific soil quality indices. We conclude that imaging NIRS enables the direct mapping of some soil properties and soil threats, but that further developments to solve several technological limitations identified are needed before it can be used for soil quality assessment. The robustness of laboratory NIRS for soil quality assessment allows its implementation in soil monitoring networks. However, its routine use requires the development of international soil spectral libraries that should become a priority for soil quality research.

Résumé

Les processus de dégradation des sols ont fortement augmenté au cours des dernières décennies. Des mesures sont progressivement mises en place afin d'évaluer et de limiter l'impact des principales menaces qui ont déjà provoqué une diminution préoccupante de la qualité des sols. Des méthodes efficaces et standardisées de suivi de la qualité des sols sont donc indispensables, mais les nombreuses propriétés impliquées dans la qualité des sols compliquent son évaluation rigoureuse. L'objectif de cette revue est d'examiner le potentiel de la spectroscopie proche infrarouge (SPIR) comme outil rapide de caractérisation de la qualité des sols. Nous dressons d'abord l'inventaire des propriétés du sol liées à sa qualité qui sont prédictibles par des mesures SPIR en laboratoire. Le potentiel de l'imagerie embarquée SPIR (satellite, avion) est également abordé. Nous réalisons ensuite une synthèse des applications utilisant la réflectance spectrale des sols comme mesure intégrée de leur qualité, depuis la classification de sites selon leur état de dégradation jusqu'à la prédiction d'indices spécifiques de qualité du sol. Nous concluons que l'imagerie SPIR permet de cartographier quelques propriétés et menaces pesant sur les sols, mais les limites technologiques relevées exigent d'importants développements pour en faire un outil robuste d'évaluation de la qualité des sols. La fiabilité de la technique SPIR par mesures en laboratoire permet sa mise en œuvre rapide dans les réseaux de mesures de la qualité des sols. Toutefois, son utilisation en routine nécessitera le développement de bibliothèques spectrales internationales, qui devrait constituer une des priorités de recherche sur la qualité des sols.

Introduction

In a technology-governed and energy-intensive world, degradation of soil conditions has become a widespread problem with negative consequences for both agricultural, natural ecosystems and urban areas (Wander & Drinkwater, 2000; Biasioli *et al.*, 2005). Scientific and political awareness of soil has emerged progressively during the second part of the 20th century (Breure, 2004), with concerns over the sustainability of agriculture and the increasing number of contamination incidents (Eijsackers, 2004). Soil scientists started attempting to define soil quality (Larson & Pierce, 1991) and the first soil protection policy appeared in the 1970s (Eijsackers, 2004), although the concept of soil quality is still debated (Sojka & Upchurch, 1999). Nowadays, quality or vitality of soils is considered to be their long-term ability to maintain their functions, which can be summarized by a combination of different elements: Robustness, Resilience, Recovery, and structural and functional Richness (Eijsackers, 2004). Another important feature in the definition of soil quality is its positive interaction with the external environment (Larson & Pierce, 1991), which is often described as the many ecosystem services provided by soils to human life (Lavelle *et al.*, 2006).

Practical assessment of soil quality remains a challenging task since it requires the integrated consideration of key soil properties involved in soil functioning and their variation in space and time (Doran & Parkin, 1994; Doelman & Eijsackers, 2004). Soil monitoring is thus essential for the early detection of changes in soil quality (Morvan *et al.*, 2008). However, selecting monitoring variables remains difficult (Zornoza *et al.*, 2007) as the establishment of any *a priori* criterion and threshold for soil quality can be considered subjective since it relies on expert opinions (Sojka & Upchurch, 1999; Andrews *et al.*, 2004; Velasquez *et al.*, 2007).

Recent studies have proposed several conceptual frameworks for monitoring soil quality (Andrews *et al.*, 2004; Velasquez *et al.*, 2007). They usually share a common first step with the choice of a minimum data set (MDS, Table 1) made of chemical, physical, and biological properties essential in terms of soil functioning (Doran & Safley, 1997). Then soil attributes are selected from

the MDS for their suitability to assess a particular soil function (Andrews *et al.*, 2004), a specific soil ecosystem service (Velasquez *et al.*, 2007), or a key threat to soils (Morvan *et al.*, 2008). Each indicator measure is further normalized to a unitless score, and finally integrated into a global soil quality index value (Andrews *et al.*, 2004; Velasquez *et al.*, 2007), fulfilling Haberern's wish (1992). However, since many soil analyses are involved, monitoring such soil quality indices at the regional or global scale remains too expensive and time consuming when using standard procedures for the measurement of soil properties. This statement is particularly true when considering the five- to ten-year sampling interval required by soil monitoring networks (SMN; Jolivet *et al.*, 2006) for an early detection of changes in soil quality, in order to implement policy measures to protect soils and maintain their sustainable use (Morvan *et al.*, 2008).

By contrast, near infrared reflectance spectroscopy (NIRS) is a rapid, non-destructive, reproducible and cost-effective analytical method involving diffuse reflectance measurement in the near infrared region (NIR; 780-2500 nm; Sheppard *et al.*, 1985). Reflectance signals result from vibrations in C–H, O–H, N–H chemical bonds, and provide information about the proportion of each element in the analysed sample (Ciurczack, 2001). Absorbances in the NIR are weak since they concern overtones or combinations of fundamentals (Figure 1; Wetzel, 1983). Although a qualitative interpretation of NIR spectra through visual analysis can be achieved (Stoner & Baumgardner, 1981), direct quantitative prediction of soil characteristics is almost impossible because soil constituents interact in a complex way to produce a given spectrum. The quantification of the property of interest is therefore usually done with statistical models and is the subject of the discipline called *Chemometrics*. An overview of the use of chemometrics in spectroscopy, its history and main concepts has been published by Geladi (2003). The quantitative analysis of NIRS data may be conducted in two ways, both requiring the implementation of multivariate statistics (Burns & Ciurczack, 2001). Firstly, clustering techniques can be used to discriminate samples or to detect changes in sample properties (Albrecht *et al.*, 2008). Secondly, a set of regression methods allows the prediction of many properties of unknown samples using calibration equations that relate spectral information to sample properties measured by conventional methods, within a calibration subset (Martens & Dardenne, 1998; Chang *et al.*, 2001).

Near infrared analysis is a well-known tool that has been utilized in many disciplines such as food science and pharmacology. Although its potential has been recognized by soil scientists for a few decades (Bowers & Hanks, 1965; Stoner & Baumgardner, 1981; Dalal & Henry, 1986), the use of NIRS for soil applications remains poorly developed (Ben-Dor *et al.*, 2008a). Nevertheless, the appearance of portable and flexible NIR devices could provide the large amount of spatial data required for monitoring soil conditions or modelling soil processes.

One can basically distinguish three types of NIRS measurements for soils (although other classifications are possible): (i) laboratory measurements, (ii) proximal sensing measurements and (iii) remote sensing measurements. The two latter techniques are able to collect spectral data *in-situ* and are therefore usually exploited to map soil properties (Barnes *et al.*, 2003). Many authors report the development of spectral sensors mounted on tractors (Shonk *et al.*, 1991; Sudduth & Hummel, 1993; Mouazen *et al.*, 2007). These systems are generally used in precision agriculture to manage the quantity of nutrient inputs into soils (Adamchuk *et al.*, 2004). Proximal sensing may also include hand-held measurement, which is used as a fast tool to monitor soil properties *in-situ* (Kooistra *et al.*, 2001; Udelhoven *et al.*, 2003; Stevens *et al.*, 2008). Ben-Dor *et al.* (2008b) recently presented a NIR sensing device able to collect *in-situ* 3D spectral data through an entire soil profile, allowing a rapid and objective soil classification. Remote sensing of soil properties has been attempted using aerial photographs (e.g. Chen *et al.*, 2000), multispectral (e.g. Galvão *et al.*, 2001) or hyperspectral images (also called imaging spectroscopy; e.g. Ben-Dor *et al.*, 2002). Imaging spectroscopy differs from multispectral imaging in its greater number of wavebands, enabling precise recording of the spectrum and a detailed analysis of spectral properties of the soil surface.

The aim of this paper is to review the most recent applications of NIRS for soil quality assessment in order to examine critically the suitability of its implementation as a tool in soil monitoring plans and networks. First, we present laboratory and imaging NIR spectrometry as tools for the quantification and mapping of many MDS variables for soil quality assessment. Then we give a brief review of studies using NIRS as an integrated measure of soil quality. These range

from global site classification to the prediction of specific soil quality indices designed to assess particular soil ecosystem services or functions. Finally we review the main research needs that could allow the implementation of laboratory NIRS for the routine assessment of soil conditions in SMN, and develop the use of imaging NIRS for the regional monitoring of soil quality.

Monitoring MDS of soil quality with NIRS

MDS information within NIR spectra of soils: insights from laboratory spectrometry

An increasing number of studies emphasise the ability of NIR analysis for the prediction of many soil attributes, including chemical, physical, and biological properties (Reeves *et al.*, 2000; Malley *et al.*, 2004; Viscarra-Rossel *et al.*, 2006). Some of these variables are key properties which were included in the first MDS for soil quality assessment published at the beginning of the 1990s (Larson & Pierce, 1991; Doran & Parkin, 1994). Since a consensus is still to be found on a MDS for soil quality, we give a list of soil chemical (Table 1a), physical (Table 1b), and biological (Table 1c) properties included in published MDS along with the predictive efficiency of NIR analysis for these properties. Most NIR regression models presented in Table 1 are based on laboratory measurements under controlled conditions, which avoid disturbing factors characterizing field measurements like soil moisture content, soil roughness and vegetation cover (Stevens *et al.*, 2008). When available, we also provide the NIR wavelengths or spectral intervals closely associated to these MDS variables of soil quality.

Regarding soil chemical properties (Table 1a), numerous authors have reported accurate NIRS predictions of soil total C and N (Al-Abbas *et al.*, 1972; Chang *et al.*, 2001; Brunet *et al.*, 2007) and pH (Chang *et al.*, 2001; Reeves & McCarty, 2001; Shepherd & Walsh, 2002). This is consistent, considering that numerous bonds between C and O, N or H absorb light in the NIR region, while pH prediction has been attributed to O–H groups (Malley *et al.*, 2004). Good

predictions for K have also been achieved using NIRS (Chang *et al.*, 2001; Confalonieri *et al.*, 2001; Shepherd & Walsh, 2002) though Malley *et al.* (2004) considered it was generally not amenable to NIRS analysis. Good NIRS predictions are less frequent for soil P and mineral N as underlined by Malley *et al.* (2004): calibrations for P and mineral N rarely perform well in soil ($R^2 = 0.4-0.5$ in general; Malley *et al.*, 2002, for P and mineral N; Chang *et al.*, 2001, and Shepherd & Walsh, 2002, for P), though good results have sometimes been obtained (Confalonieri *et al.*, 2001, and Bogrekci & Lee, 2005, for P; Cho *et al.*, 1998, for mineral N). Contradictory NIRS predictions have been reported for salt content in soil ($R^2 = 0.1-0.6$ for Chang *et al.*, 2001, and Malley *et al.*, 2002; $R^2 = 0.1-0.8$ for Farifteh *et al.*, 2008; but $R^2 = 0.7-0.8$ for Dunn *et al.*, 2002) and for electrical conductivity ($R^2 = 0.4-0.6$ for Dunn *et al.*, 2002; but $R^2 = 0.7$ for Malley *et al.*, 2004). Very contradictory results have been reported regarding NIRS prediction of soil heavy metal content depending on the element, and apparently, on the site and on the reference method too. For instance, some authors reported good predictions of Cd, Co and Zn (Kooistra *et al.*, 2001, Wu *et al.*, 2007, and Kooistra *et al.*, 2001, respectively) while others reported poor predictions (Wu *et al.*, 2007, Malley *et al.*, 2004, and Chang *et al.*, 2001, respectively). Contradictory results have also been achieved for Cr, Cu, Ni and Pb (Malley *et al.*, 2004; Wu *et al.*, 2007). Similarly, the fate of organic pollutants in soil is an important and widespread concern, although these are not currently included in MDS of soil quality. Bengtsson *et al.* (2007) reported promising results regarding NIRS prediction of pesticide sorption to soils. Contradictory results for K, P, mineral N, salt or heavy metals may have several causes, either relating to the reference methods (e.g. prediction of extractable cations varies with the extraction method; Chang *et al.*, 2001), the nature of the studied element (e.g. spectrally distinct P-containing compounds may variably contribute to soil P content; Malley *et al.*, 2004), its concentration (e.g. below detection limits), or possible interactions with other components (e.g. water, organic matter or iron oxides; Malley *et al.*, 2004). To a larger extent, poor predictions may also result from low-quality reference data, subsampling errors (reference and spectral analyses being performed on dissimilar subsamples), heterogeneity of sample sets (optimal calibration requires limited but sufficient set heterogeneity), or inappropriate calibration (e.g. fail to improve the signal-to-noise ratio or overfitting).

There have also been attempts to predict soil physical properties using NIRS (Table 1b), which have yielded good results for soil particle size distribution (especially for clay content; Al-Abbas *et al.*, 1972; Ben-Dor & Banin, 1995a; Chang *et al.*, 2001; Morón & Cozzolino, 2003), soil moisture (Bowers & Hanks, 1965; Dalal & Henry, 1986; Ben-Dor & Banin, 1995a; Chang *et al.*, 2001), water holding capacity (Sudduth & Hummel, 1993; Zornoza *et al.*, 2008), infiltration of crusted soils (Goldshleger *et al.*, 2002), and maximum temperatures reached by burned soils (Guerrero *et al.*, 2007), but not for the size distribution of water-stable aggregates (Chang *et al.*, 2001). Particle size effects on light transmission and reflection, and strong absorption features exhibited by water, explain the accurate predictions for texture and moisture, while poor performance regarding aggregate distribution has been attributed to inappropriate procedures (Chang *et al.*, 2001).

NIRS prediction of soil biological properties has often yielded good results (Table 1c), as reported for microbial biomass (Reeves *et al.*, 1999; Chang *et al.*, 2001; Ludwig *et al.*, 2002), soil respiration (Palmborg & Nordgren, 1993; Chang *et al.*, 2001; Ludwig *et al.*, 2002), potentially mineralizable N (Chang *et al.*, 2001; Fystro, 2002; Ludwig *et al.*, 2002; Shepherd & Walsh, 2002), and even for the ratio of microbial to total organic C (Ludwig *et al.*, 2002; Cécillon *et al.*, 2008) and for the density of soil microorganisms (Zornoza *et al.*, 2008). Good predictions have been attributed to the similarity between spectral responses of most biological properties and that of soil organic C (Chang *et al.*, 2001).

Upscaling NIR assessment of soil quality: imaging spectrometry

Imaging spectrometry might yield a new dimension to the field of NIRS for the prediction of soil properties by enlarging the envelope of laboratory spectrometry spatially (Ben-Dor *et al.*, 2008a). This wider spatial dimension can be obtained using visible-NIR (Vis-NIR) spectrometers onboard either airborne or satellite. Remotely-sensed hyperspectral satellite data offer a synoptic view and a repetitive coverage which are two important advantages compared to ground observations and hyperspectral airborne data. While the contribution of multispectral satellite data in the analysis of

soil properties has been already investigated (e.g. Ben-Dor & Banin, 1995b; Nanni & Demattè, 2006), the use of hyperspectral satellite data for soil property prediction remains poorly studied.

Using airborne hyperspectral sensors, fairly good to good NIRS predictions have been achieved for soil organic C ($R^2 = 0.74-0.9$, Ben-Dor *et al.*, 2002; Selige *et al.*, 2006; Stevens *et al.*, 2008; De Tar *et al.*, 2008; Patzold *et al.*, 2008), total N ($R^2 = 0.92$, Selige *et al.*, 2006), clay content ($R^2 = 0.61-0.71$, Selige *et al.*, 2006; De Tar *et al.*, 2008; Lagacherie *et al.*, 2008), sand or silt content ($R^2 = 0.75-0.95$, Selige *et al.*, 2006; De Tar *et al.*, 2008), soil moisture ($R^2 = 0.64$, Ben-Dor *et al.*, 2002), Cation Exchange Capacity ($R^2 = 0.66-0.67$, Ben-Dor *et al.*, 2002; De Tar *et al.*, 2008), pH ($R^2 = 0.52-0.61$, Ben-Dor *et al.*, 2002; De Tar *et al.*, 2008) and Ca, Mg, Na, Cl, K, P ($R^2 = 0.58-0.7$, De Tar *et al.*, 2008).

Weng *et al.* (2008), obtained good predictive models for soil salt content in the Yellow river delta using the Hyperion satellite hyperspectral sensor ($R^2 = 0.78$). By contrast, relatively low prediction accuracy was reported for soil organic C with the same sensor ($R^2 = 0.51$, Gomez *et al.*, 2008). This lower accuracy was assumed to be the result of several factors: (i) the low signal-to-noise ratio of Hyperion spectra, (ii) the low spatial resolution (30 m) which induces mixing problems, and (iii) the relatively low level of carbon in the soils.

Despite the potential of imaging spectrometry for mapping soil properties within the MDS, there are still several limitations, which may preclude the use of such technique to address real problems. These limitations can be related to: (i) the measure itself (sensing device and measuring environment), and (ii) differences in sample preparation and conditions which cannot be controlled in the field.

The first category of limitations is caused by the distance between the sensor and the soil surface. Appropriate correction techniques are required to handle the effects of varying light and atmospheric conditions on the signal. A precise georeferencing of the image is also needed to attribute correctly each soil sample to a pixel. A good introduction to the processing and geometric/atmospheric correction of hyperspectral data can be found in Aspinall *et al.* (2002). Ben-Dor *et al.* (2004) examined the accuracy of several correction methods to retrieve the true

reflectance values from imaging spectroscopy data. They found a difference of up to 40% between modelled and true reflectance information at specific wavelengths, depending on the correction method used and variability in atmospheric conditions. When using a 'top-down' approach (i.e. detection of a given soil property based on field sampling) and when the spatial extent of hyperspectral images is small, atmospheric effects may be constant over the study area and a particular object will appear similar across the image (Aspinall *et al.*, 2002). However, when the analysis is conducted over larger images or when a 'bottom-up' approach is used (i.e. detection of a given soil property based on laboratory-based spectral libraries), accurate atmospheric correction is crucial. Another limitation is the relatively low signal-to-noise ratio of hyperspectral data compared with laboratory data due to a low integration-time over the target area. Chabrillat *et al.* (2002) demonstrated for instance that the detection of expanding clays may be degraded because the spectral feature used to identify the type of clay may be of the same amplitude as the noise in the data. By comparing airborne hyperspectral HyMap and AVIRIS data over the same area, Chabrillat *et al.* (2002) also showed the influence of the spectral and spatial configuration of the sensor. The coarser spectral resolution of HyMap compared to AVIRIS in the 2000-2500 nm spectral region masked partly the doublet spectral feature at ~2150 nm related to clay type and reduced the effectiveness of the classification. Conversely, the higher spatial resolution of HyMap allowed obtaining purer spectral end-members (i.e. spectra not influenced by other soil constituents or by soil surface characteristics) in more heterogeneous sites. Spatial resolution is thus a matter of importance when the studied soil property occurs in a patchy way or is affected by a strong spatial variability (e.g. soil crusting).

The second category of limitations is related to the spatial and temporal variability of soil surface conditions. This variability often reduces the accuracy of the prediction of soil properties by chemometric techniques in areas having different surface conditions than the ones in the calibration set (Stevens *et al.*, 2008). Some of the properties that are subject to variation in time and space are: moisture content, degree of soil crusting, particle-size, soil roughness, vegetation or crop residue cover. In the study of Kooistra *et al.* (2003), soil moisture and vegetation cover were identified as the main causes of the loss of accuracy between field and laboratory spectra.

The effects of soil roughness on bidirectional reflectance behaviour have been studied in detail (see e.g. Cierniewski & Courault, 1993). Usually, rough soils present highest reflectance values when measured from the direction of the illumination source and lower reflectance values in positions away from this peak. Since remote sensors record the soil surface under varying illumination and viewing angles, this phenomenon induces a spectral variability not specifically related to the studied property. Another constraint of importance is the vegetation/residue cover, partly masking the soil signal. Bartholomeus *et al.* (2007) showed that even a small vegetation cover (5%) leads to large variations in the estimations of soil parameters. Imaging spectrometry campaigns must therefore be organized only in arid/semi-arid regions or when the soil has been recently tilled. Finally, imaging spectroscopy is only able to measure the reflectance within the first few millimetres of the surface and can therefore not predict a given property for the entire soil profile. As a consequence, such a method of data acquisition may be of little interest when strong vertical gradients in soil properties occur.

An alternative solution: the rough quantification of MDS variables

As presented above, NIR spectra of soil samples contain much information relevant to soil quality, and multivariate regressions of NIR spectra from laboratory and imaging spectrometry can accurately predict several properties of MDS. However, soil quality does not always need to be precisely quantified. Many industrial or agricultural applications only require a classification of soil condition with respect to a critical test value for key properties. Shepherd & Walsh (2002) were the first to propose the use of laboratory NIR analysis for the discrimination of soils falling above or below specific cut-off values for most properties related to soil fertility. They showed that soil samples could be roughly discriminated using classification trees even for properties like exchangeable K and extractable P which are poorly predicted by regression models. These promising findings were further confirmed by Cohen *et al.* (2005a) on an extensive data set of quality parameters for wetland soils, including soil microbiological attributes.

Integrated assessment of soil quality with NIR analysis

NIRS as a fingerprint of global soil conditions

Since NIR spectra of soils reflects a set of soil quality attributes like organic matter content and some chemical and biological properties, some researchers have hypothesized that laboratory NIRS could probably be used to discriminate clusters of soil samples differing in their “global” quality. Velasquez *et al.* (2005) first tested the use of principal component analysis (PCA) and discriminant analysis to separate soils from different land uses. This strategy successfully discriminated clusters of sites depending on land-use type, and co-inertia analyses revealed significant relationships between NIR spectra and various physico-chemical properties of soil samples. The authors also identified NIR wavelength intervals characteristic of the soil-use systems. This PCA strategy was further applied by Cécillon *et al.* (2009) on a NIR spectral data set of Mediterranean topsoils and earthworm casts collected in areas affected by wildfire (Figure 1). Soil samples and biogenic structures were well separated by PCA on NIR spectra, depicting the influence of earthworms on soil quality, as previously demonstrated by Hedde *et al.* (2005). Furthermore, a strong effect of wildfire on NIR spectra could also be identified in this PCA. This striking result was the first illustration of the use of laboratory NIRS to estimate the effect of an ecological factor (wildfire) on soil conditions. Odlare *et al.* (2005) coupled PCA of NIR soil spectra and geostatistics to map spatial variation of soil properties. Since principal components of PCA synthesize information on global soil condition, such an approach is interesting for mapping soil quality in precision farming, or for the quantitative spatial assessment of polluted areas in environmental remediation procedures.

Other studies have focussed on the use of laboratory NIR analysis as an integrated tool for the assessment of global soil quality. Using a holistic definition of soil quality, Vågen *et al.* (2006) aggregated ten commonly used agronomic indicators of soil quality (pH, organic C, total N, P, Ca, Mg, K, CEC, clay, silt) and developed ordinal soil condition classes (poor, average, good), which

were used to identify spectral wavebands that could diagnose soil condition. They found that five wavelengths were related to their soil quality index: relative reflectance at 570, 1410, 2040 and 2390 nm were negatively correlated with soil condition class whereas relative reflectance at 1940 nm (which is almost certainly due to O–H bond of water) was positively correlated with soil condition class. The authors computed a soil fertility index (SFI), calibrating the membership of the three soil condition classes to reflectance spectra of soils using a proportional odds ordinal logistic regression model. Finally, the SFI was successfully applied to the spatial representation of global soil quality based on remote sensing satellite imagery. Awiti *et al.* (2008) applied the same proportional odds ordinal logistic regression modelling technique to chronosequence classes of forest-cropland plots and the 10 first principal components calculated from PCA of soil NIR spectra. Using this strategy, the authors could determine three global soil condition classes (good, average and poor) which were then used for the successful classification of soils from unknown sites. Cohen *et al.* (2006) used another NIR-based approach of global soil quality. They combined ordinal logistic regression and classification trees of soil NIR spectra to discriminate between ecological condition categories. Using classification trees, they identified key spectral regions for ecological condition classification: 2200–2300 nm, 1100–1200 nm, and 500–600 nm. They concluded that site classification with soil reflectance data was more efficient than with biogeochemical data, especially for the discrimination of severely degraded sites. Soil NIR spectra thus provide an effective tool for rapid condition diagnosis of soils and ecosystems (Cohen *et al.*, 2006).

NIR-based diagnostics of specific soil quality

Global assessment of soil conditions with NIRS, as presented above, enables a rapid tracking of states of soil quality or of its changes after a disturbance. In addition, successful classifications of sites have been built regarding land-use type or global soil condition classes. However, soil quality policies usually address specific management goals such as productivity, waste recycling or

environmental protection (Andrews *et al.*, 2004). Thus, methodologies for soil quality assessment should be able to measure specific soil functions or soil ecosystem services associated with these management goals. Recently, the European Commission (2006) identified several key threats to European soils, including soil erosion, soil contamination and loss of organic matter. An important objective of soil quality research is thus to provide economically realistic tools for the monitoring of these threats (Morvan *et al.*, 2008).

Following the widespread use of remote sensing in environmental management, the suitability of imaging spectrometry for specific soil quality assessment has been tested since the 1990s and was recently reviewed by Ben-Dor *et al.* (2008a, see references therein). The authors listed promising results of imaging NIRS regarding the quantification and mapping of some specific soil threats. Salinisation of soils has been fairly extensively studied using airborne reflectance data (HyMap, DAIS-7915). Qualitative indicators of soil erosion have also been mapped using airborne AVIRIS imaging spectrometry, with an accuracy of about 80%, which was superior to that achieved using Landsat-TM imagery. HyMap airborne data have been used to estimate the distribution of sludge containing large concentrations of heavy metals, demonstrating the potential of NIRS imaging to map soil contamination and monitor environmental remediation procedures. Finally, airborne reflectance data (AVIRIS, HyMap) in the presence of significant vegetation cover and NIRS satellite imaging (ASTER, wavebands between 2145 and 2430 nm) have been shown reliable for mapping soil swelling. These results could be useful to engineers for construction planning, decision makers for better management of the environment, and farmers in allocating hazardous areas like floods and erosion sites (Ben-Dor *et al.*, 2008a).

The application of laboratory spectrometry for the specific assessment of soil quality started in the 2000s. Cohen *et al.* (2005b) presented the first application for the rough assessment of a specific soil threat. They showed that NIRS clearly outperformed a frequently used empirical model for classifying sites according to soil erosion status. They used classification trees to provide an objective definition of degraded and intact soil conditions and developed NIRS-based screening models calibrated with reliable visual observations of degraded sites. These NIRS classification models were found efficient in discriminating three degradation classes (intact, moderate and

severe erosion). This rough assessment of a soil threat could be a useful tool for characterizing site conditions prior to irreversible degradation (Cohen *et al.*, 2005b).

However, an important goal for soil monitoring is the detection of small changes in specific key threats, functions or services over space and time. Thus, most recent soil quality indicators have been designed to achieve these ends (Andrews *et al.*, 2004; Velasquez *et al.*, 2007), but their implementation in soil monitoring networks remains too expensive and time consuming to be economically realistic using conventional soil analyses.

Recent research has focussed on the quantitative prediction of specific and targeted soil quality indices with laboratory NIRS. Shepherd & Walsh (2007) presented some preliminary tests of indices designed to assess particular soil functions or threats such as soil fertility, soil erosion rate, soil erodibility, soil infiltration capacity, and plant growth potential. Their specific spectral indicators were based on the Mahalanobis distance in the principal component space built using a library of soil reflectance spectra. Cécillon *et al.* (2009) recently proposed a tentative approach based on the direct prediction of specific soil quality indices related to soil ecosystem services using laboratory NIRS. The accuracy of three soil quality indicators derived from the general indicator of soil quality (GISQ; Velasquez *et al.* 2007) was tested on the impact of wildfire disturbance (time since last fire) and soil engineering activity of earthworms (topsoil *versus* casts samples). For each sample, conventional analyses related to three soil ecosystem services were performed. Organic matter storage was assessed through organic C and total and mineral N contents, nutrient supply through pH and exchangeable cations (Ca, Mg, K, Na, CEC), and biological activity through a set of microbiological parameters (microbial C, two extracellular enzymes, potential denitrification and microbial C to organic C ratio). Three specific indicators (SI) of soil quality, reflecting the provision of these soil ecosystem services, were then computed using the GISQ approach (Velasquez *et al.*, 2007). Higher SI values indicate more ecosystem services produced, thereby an improved soil quality (Velasquez *et al.*, 2007). The predictive ability of NIR analysis for the three SI was assessed with partial least squares regression (PLSR; Tenenhaus, 1998). PLSR models for the three SI reached “reasonable” statistics (Williams, 1993), with cross-validated coefficients of determination (Q^2) above 0.90 and ratio of performance to deviation (RPD)

above 2.8 (Figure 2; Cécillon *et al.*, 2009). These results are the first attempt to predict specific soil quality indices with laboratory NIRS. They open a new pathway for soil quality research, as a simple scan of a soil sample with a NIR spectrometer can provide quantitative information on the provision of a given soil ecosystem service. The same strategy could probably be applied for the assessment of a soil function or a soil threat critical for management goals.

Implementing this cost-effective strategy could have wide implications for the spatial coverage and the sampling frequency of soil monitoring networks (SMN). Existing SMN sites and data could be used for the regional calibration of soil quality indices. Then a quantitative assessment of soil quality could be performed at the field scale depending on the end-user or land manager's needs. The sampling frequency of SMN could also be increased enabling a seasonal assessment of soil quality, which is crucial for the early detection of changes in soil conditions.

Research needs towards NIR monitoring of soil conditions

Soil spectral libraries: enabling the implementation of laboratory spectrometry in SMN

Hitherto, NIRS has mainly been applied to soils at the field or the landscape scale, and no generalization can be inferred from regression models obtained with such local studies. One of the main gaps in effective monitoring of soil quality with NIRS is the building of NIRS-based regression models capable of assessing soil conditions at the regional scale across various soil types. Shepherd & Walsh (2002) presented a new approach allowing the regional quantification of many soil properties with laboratory spectrometry. They proposed the use of soil spectral libraries as a tool for building risk-based approaches to soil evaluation. In the spectral library approach, soil properties are measured conventionally for a selection of soils representative of the diversity of the studied region, and then calibrated to soil reflectance spectra. Usually, the size of the calibration sample set is increased until calibrations are found to be sufficiently accurate for user

requirements. It is then possible to predict the soil properties for new samples that belong to the same population as the library soils. Soils that are poorly described in the library can be further characterized (conventionally) and added to the calibration library (Shepherd & Walsh, 2002). Brown *et al.* (2006) applied the soil spectral library strategy using more than 4×10^3 soil samples selected from all 50 US states, two tropical territories and 36 different countries in Africa, Asia, the Americas and Europe. They obtained satisfactory predictive efficiency for various soil physical and chemical properties and concluded that calibrations sufficient for many applications might be obtained with large but obtainable soil spectral libraries (10^4 – 10^5 samples). Genot *et al.* (2007) worked with a spectral library of ca. 10^3 soil samples representative of the Walloon region (Belgium) and obtained accurate predictions for the soil properties studied (organic C, total N, clay content and CEC). Their work now allows the routine application of laboratory NIRS by the five laboratories providing fertility advice in this region. All applications of soil spectral libraries used advanced multivariate regression techniques to infer soil properties from NIR spectra. Shepherd & Walsh (2002) and Brown *et al.* (2006) worked respectively with multivariate adaptive regression splines (MARS), and boosted regression trees (BRT), two non-linear multivariate techniques. Genot *et al.* (2007) used an improvement of the PLSR algorithm (PLS-Local; Shenk *et al.*, 1997) which matches the sample to be predicted using a small homogeneous group of spectrally similar samples selected from a calibration library. These advanced regression techniques clearly outperformed the classical PLSR approach which is often not on its own an optimal solution for processing soil spectra, especially with large datasets and a wide range of values (Cécillon *et al.*, 2008; Fernández Pierna & Dardenne, 2008).

All these promising results underline the urgent need to build a universal and standardized soil spectral library. Viscarra Rossel (2008) and colleagues from the International Soil Spectroscopy Group (<http://groups.google.com/group/soil-spectroscopy?hl=en>) are currently trying to implement such a spectral library for basic soil properties (e.g. organic C, clay content). This huge task sounds feasible for soil chemical properties using existing samples from SMN. When built, it should be possible to compute and monitor some of the specific soil quality indices presented above (e.g. organic matter storage, nutrient supply). However, the current lack of data for many MDS variables

of soil quality (especially physical and biological properties) could compromise the rapid construction of a universal soil spectral library for the global assessment of soil quality or the specific assessment of soil threats like soil erosion, contamination, or decline in soil biological activity and diversity. The soil spectral library approach for the quantification of soil quality might thus not be successful until the calibration of all MDS variables to soil reflectance spectra has been achieved, which will be difficult.

Furthermore, building NIR spectral libraries for soils raises several problems. The first problem relates to the fact that NIR spectra show subtle variations even when obtained on supposedly identical instruments. This is even more of a problem with spectra from different makes and models of instruments, or those from instruments based on different principles (diode arrays versus Fourier transform or gratings, *etc.*). The systematic differences between spectra from different instruments can make combining spectra useless for developing calibrations. To overcome these problems, chemometric procedures known as calibration transfer (e.g. Shenk *et al.*, 1985) are used to make spectra from different instruments appear the same. Much research still needs to be done so as to achieve comparability between instruments used for soil spectral measurements. The second related problem is the question of whether the measures of soil attributes included in the spectral libraries, particularly biological measures, obtained at different laboratories, are the same or not. When the two problems are combined, spectral libraries lose much of their value. These problems, while known and discussed greatly in other areas of NIRS (see e.g. Cen & He, 2007), do not seem to have received much press for soils.

McBratney *et al.* (2006) proposed an alternative approach that links soil diffuse reflectance spectroscopy with an inference system to predict soil functional properties which are difficult and expensive to measure directly. They measured soil spectra to estimate various basic soil properties which were then used to infer the desired soil functional property *via* pedotransfer functions. This approach could be promising for the assessment of soil conditions, but reliable pedotransfer functions for global or specific soil quality are not sufficiently developed.

Compared to laboratory spectroscopy, imaging spectrometry has, at the present time, some difficulties in producing reliable and robust predictions for routine soil analysis. A large part of the problem is technological (signal-to-noise ratio, spatial and spectral resolution, *etc.*) or a matter of institutional/scientific will (training of scientists, finding potential end-users) and beyond the scope of this paper (see e.g. Ben-Dor *et al.*, 2008a).

However, some progress can be rapidly achieved by applying more efficient analysis tools. The simplest solution to the problem of spatial variability in soil surface conditions is to record the surface conditions of the soil samples used in the calibration set and restrict the prediction to similar pixels (e.g. based on the Mahalanobis distance). Including a covariant such as soil moisture or roughness in the multivariate regressions is another solution, which requires the measurement of the disturbing factor over the entire study area. The recent convergence of several new measuring technologies aiming to map soil properties (e.g. synthetic aperture radar imagery) enables the investigation of such strategies in the mid-term. As presented above regarding laboratory spectrometry, the stability of the calibrations may also be improved by using more efficient chemometric approaches. For instance, the implementation of the PLS-Local algorithm with hyperspectral data would improve the accuracy, by using samples in the calibration set with surface conditions corresponding to the ones of the pixel to be predicted, providing that the spectral library would represent perfectly all surface conditions in the study area. Marx & Eilers (2002) have developed a multivariate technique – called penalized signal regressions – that forces the regression coefficients to vary smoothly across wavelengths. It allows the effects of noisy features in the spectral data to be removed from calibrations and yields more robust calibrations in general. Bartholomeus *et al.* (2008) proposed to use spectral indices (e.g. $1 / [\text{slope } 2138\text{-}2200 \text{ nm}]$), which can be easily related to the biochemical composition of the soil samples and show a greater stability.

Conclusions

This review has demonstrated that near infrared reflectance spectra contain much information related to soil quality. Using laboratory NIRS, good predictions can be achieved for many chemical and some physical and biological properties involved in soil conditions. Imaging NIRS can predict some soil chemical properties related to soil quality. Its ability to cover large surfaces in a single flight campaign and thus produce a complete picture of surface soil properties of bare soils represents a clear opportunity for monitoring. However, several technological limitations will delay its routine use for quantifying a MDS of soil quality.

Soil NIR spectra can be used as an integrated measure of soil quality, so as to classify sites according to their global degradation status or for monitoring the effect of an ecological factor on soil quality. NIRS also opens a new way for soil quality assessment, as reliable quantification of particular soil functions, ecosystem services, or threats can be evaluated from a flight campaign or a simple NIR scanning of a soil sample. Implementing this specific approach to soil quality with laboratory and imaging NIRS will provide powerful tools to address the specific management goals of soil quality policies. Laboratory NIRS offers a low-cost solution for soil quality monitoring networks which could allow an increase in their spatial coverage and an increase in their sampling frequency. Imaging NIRS provides an interesting solution for the spatial assessment of some specific soil threats in environmentally sensitive areas.

An urgent research need is the development of international soil spectral libraries that will improve the predictive ability of NIRS for soil quality attributes whatever the soil type. Coupling NIR spectral libraries with other diffuse reflectance measurements of soils, such as mid-infrared reflectance spectra, will probably be the next step towards spectral sensing of soil quality worldwide.

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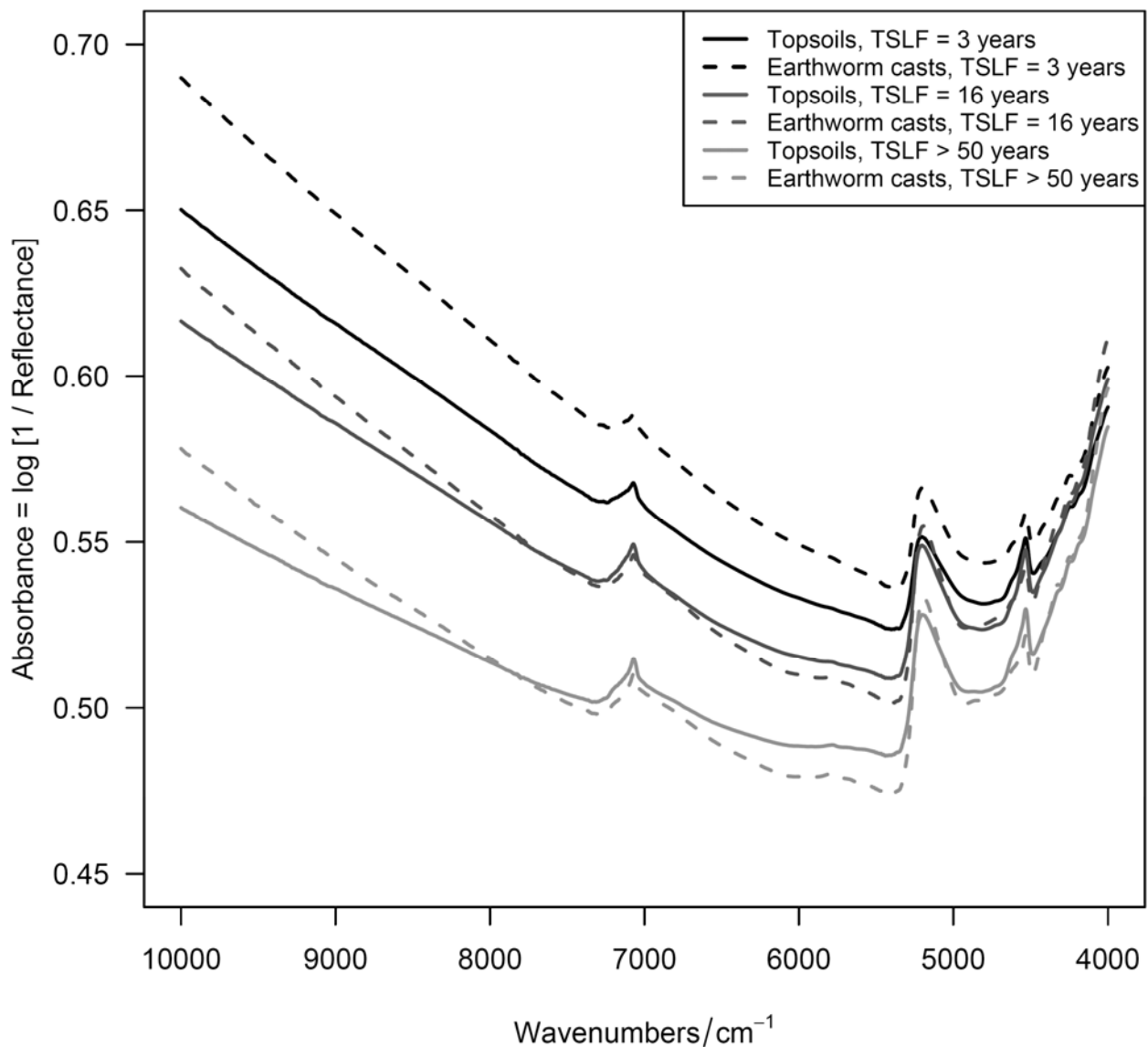


Figure 1 Weak absorption peaks in NIR spectra of topsoils (0-5 cm) and earthworm casts collected in French Mediterranean areas affected by wildfire (Cécillon *et al.*, 2009). Each spectrum is an average of samples originating from five to ten plots.

Wavelengths (nm) can be computed from wavenumbers (cm^{-1}) with the following formula:

$$\text{Wavelength} = [1 / \text{Wavenumber}] \times 10^7$$

Abbreviation: TSLF = time since last fire

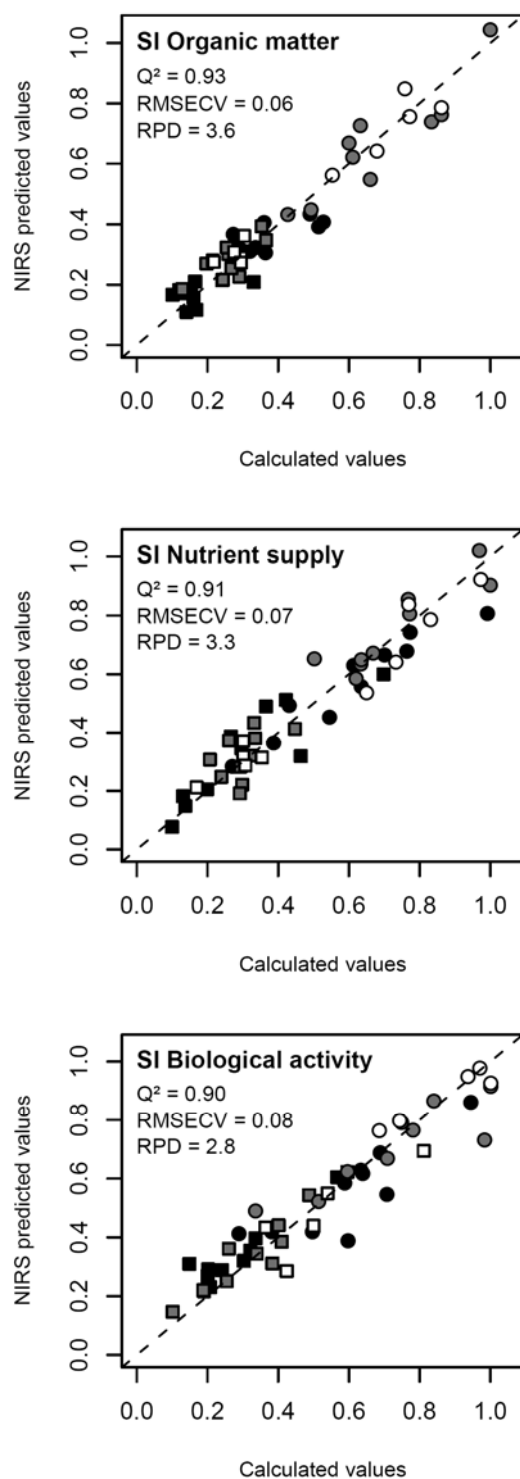


Figure 2 Predictive efficiency of laboratory NIRS for specific indices (SI) of soil quality related to three soil ecosystem services in French Mediterranean areas (modified from Cécillon *et al.*, 2009). Squares correspond to topsoil samples and circles to earthworm casts. Black, grey and white symbols correspond to sites where time since last fire was 3, 16 and > 50 years, respectively. The dashed lines represent the 1:1 lines.

Abbreviations: Q^2 = cross-validated R^2 ; RMSECV = root mean squared error of cross-validation RPD = ratio of performance-to-deviation (calculated as $RPD = SD \text{ RMSECV}^{-1}$); SD = standard deviation of calculated SIs

TABLES

Table 1a Predictive efficiency of NIRS for MDS regarding soil chemical variables and associated soil functions, ecosystem services or threats.

MDS variable ¹	Soil functions ²	Soil ecosystem services ³	Soil threats studied in SMN ⁴	NIRS predictive efficiency ⁵	Associated NIR wavelengths and references
Organic C	Nutr. Cycling ⁶ ; filter-buffer; biodiv-habitat ⁷	Nutr. Cycling ⁶ ; climate regul ⁸ ; detox ⁹	SOM ¹⁰ decline	Good	1744, 1870, 2052 nm (Dalal & Henry, 1986); 1955-1965, 2215, 2265, 2285-2295, 2315-2495 nm (Henderson <i>et al.</i> , 1992); 2218, 2350 nm (Salgó <i>et al.</i> , 1998); 2200 nm (Confalonieri <i>et al.</i> , 2001); 1109, 1232, 1414, 1522 nm (Mouazen <i>et al.</i> , 2007); 1420, 1900-1950, 2040-2260, 2440-2460 nm (Rinnan & Rinnan, 2007); 1130, 2410 nm (Terhoeven-Urselmans <i>et al.</i> , 2008)
Total and organic N	Nutr. Cycling ⁶ ; filter-buffer; biodiv-habitat ⁷	Nutr. Cycling ⁶ ; climate regul ⁸ ; detox ⁹	SOM ¹⁰ decline	Good	For total N: 1702, 1870, 2052 nm (Dalal & Henry, 1986); 1726, 1826, 2038 nm (Morra <i>et al.</i> , 1991)
PH	Nutr. Cycling ⁶ ; filter-buffer; biodiv-habitat ⁷	Nutr. Cycling ⁶	Contamination	Mid	
Electrical conductivity	Nutr. Cycling ⁶	Nutr. Cycling ⁶	Desertification; salinisation	Mid	
Mineral N, P, K	Nutr. Cycling ⁶	Nutr. Cycling ⁶	Contamination	Mid	For NH ₄ : 1510-1650 nm (Murray & Williams, 1990); for total P: 2021-2025, 2081-2084 nm (Bogrekci & Lee, 2005); 2240-2400 nm (Velasquez <i>et al.</i> , 2005)
Heavy metal content	Nutr. Cycling ⁶ ; resilience; filter-buffer	Nutr. Cycling ⁶ ; detox ⁹	Contamination	Mid	For Cu: ca. 900, 1300, 1500 nm (Gaffey & Reed, 1987); for Cd and Zn: 1050, 1400, 1850, 2150, 2280, 2400, 2470 nm (Kooistra <i>et al.</i> , 2001)
Salt content	Nutr. Cycling ⁶		Desertification; salinisation	Mid	For NaCl: 1930 nm; for KCl: 1430 nm; for MgSO ₄ : 1480 nm; for Na ₂ SO ₄ : 1825 nm; for MgCl ₂ : 1925 nm (Farifteh <i>et al.</i> , 2008)

¹ modified from Doran & Parkin, 1994; ² after Andrews *et al.*, 2004; ³ after Lavelle *et al.*, 2006; ⁴ after Morvan *et al.*, 2008; ⁵ based on validation statistics (R², standard error of prediction); ⁶ nutrient cycling; ⁷ biodiversity and habitat; ⁸ climate regulation; ⁹ detoxification; ¹⁰ soil organic matter.

Table 1b Predictive efficiency of NIRS for MDS regarding soil physical properties and associated soil functions, ecosystem services or threats.

MDS variable ¹	Soil functions ²	Soil ecosystem services ³	Soil threats studied in SMN ⁴	NIRS predictive efficiency ⁵	Associated NIR wavelengths and references
Soil loss	Physical support; water relations	Erosion control	Soil erosion	Poor	For infiltration of crusted soils: ca. 1400, 1450, 1900, 2200 nm (Goldshleger <i>et al.</i> , 2001, 2002)
WSA ⁶	Physical support; water relations	Erosion control; climate regul ⁷	Soil erosion; SOM ⁸ decline	Mid	
Soil texture	Physical support; biodiv-habitat ⁹ ; filter-buffer	Erosion control; detox ¹⁰	Compaction; soil formation	Mid	For clay: 2200 nm (Ben-Dor & Banin, 1995a); 1700 nm (Viscarra Rossel & McBratney, 1998); 1901, 1912 nm (Islam <i>et al.</i> , 2003); 2206 nm (Lagacherie <i>et al.</i> , 2008); for particle size: 1323, 2021, 2081 nm (Bogrekci & Lee, 2005)
Soil structure	Physical support; biodiv-habitat ⁹ ; filter-buffer	Erosion control; climate regul ⁷ ; water supply; detox ¹⁰	Compaction; soil formation	Poor	For aggregate fractions: 1940, 2250 nm (Mutuo <i>et al.</i> , 2006)
Depth of soil and rooting	Physical support; water relations; biodiv-habitat ⁹	Erosion control; soil formation; detox ¹⁰	Soil formation	Poor	
Bulk density	Physical support; water relations	Water supply; soil formation	Compaction; SOM ⁸ decline; soil formation	Poor	
WHC ¹¹	Physical support; water relations	Water supply		Mid	
Water content	Physical support; water relations	Water supply		Good	1400, 1900, 2200 nm (Bowers & Hanks, 1965; Ben-Dor & Banin, 1995a; Demattê <i>et al.</i> , 2006); 1926, 1954, 2150 nm (Dalal & Henry, 1986); 1450, 1920 nm (Salgó <i>et al.</i> , 1998); 1450, 1950, 2500 nm (Viscarra Rossel & McBratney, 1998); 1420, 1920 nm (Confalonieri <i>et al.</i> , 2001)
Soil temperature	Water relations; nutr. Cycling ¹² ; biodiv-habitat ⁹	Nutr. Cycling ¹² ; climate regul ⁷ ; soil formation		Poor	

¹ modified from Doran & Parkin, 1994; ² after Andrews *et al.*, 2004; ³ after Lavelle *et al.*, 2006; ⁴ after Morvan *et al.*, 2008; ⁵ based on validation statistics (R², standard error of prediction); ⁶ water stable aggregates; ⁷ climate regulation; ⁸ soil organic matter; ⁹ biodiversity and habitat; ¹⁰ detoxification; ¹¹ water holding capacity; ¹² nutrient cycling.

Table 1c Predictive efficiency of NIRS for MDS regarding soil biological properties and associated soil functions, ecosystem services or threats.

MDS variable ¹	Soil functions ²	Soil ecosystem services ³	Soil threats studied in SMN ⁴	NIRS predictive efficiency ⁵	Associated NIR wavelengths and references
Microbial biomass	Nutr. Cycling ⁶ ; resilience; filter-buffer; biodiv-habitat ⁷	Nutr. Cycling ⁶ ; climate regul ⁸ ; soil formation; plant production and protection	Biodiversity decline	Good	1408, 1842, 2414 nm (Terhoeven-Urselmans <i>et al.</i> , 2008); wavelength interval 1750-2500 nm (Cécillon <i>et al.</i> , 2008)
Soil respiration	Nutr. Cycling ⁶ ; resilience; filter-buffer; biodiv-habitat ⁷	Nutr. Cycling ⁶ ; climate regul ⁸	Biodiversity decline	Good	800 (Fe oxide effect), 2030, 2180, 2200 (clay mineralogy effect), 2250, 2440, 2460 nm (Mutuo <i>et al.</i> , 2006); for basal respiration: 1836, 2274 nm (alkyl groups), 1510 nm (amino groups) (Terhoeven-Urselmans <i>et al.</i> , 2008)
Potentially mineralizable N	Nutr. Cycling ⁶ ; resilience; filter-buffer	Climate regul ⁸		Mid	
Cmic / Corg ratio	Nutr. Cycling ⁶ ; resilience; filter-buffer; biodiv-habitat ⁷			Good	Wavelength interval 1750-2500 nm (Cécillon <i>et al.</i> , 2008)
Respiration/ biomass ratio	Nutr. Cycling ⁶ ; resilience; filter-buffer; biodiv-habitat ⁷			ND	
Biodiversity	Resilience; biodiv-habitat ⁷	Soil formation; plant production and protection	Biodiversity decline	Poor	

¹ modified from Doran & Parkin, 1994; ² after Andrews *et al.*, 2004; ³ after Lavelle *et al.*, 2006; ⁴ after Morvan *et al.*, 2008; ⁵ based on validation statistics (R², standard error of prediction); ⁶ nutrient cycling; ⁷ biodiversity and habitat; ⁸ climate regulation; ND: not determined.