



Review article

Near-infrared laboratory spectroscopy of mineral chemistry: A review

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ABSTRACT

Spectroscopy is the science concerned with the investigation and measurement of spectra produced when materials interact with or emits electromagnetic radiation. Commercial infrared spectrometers were designed from the 1950's onward and found their way into the pharmaceutical and chemical industries. In the 1970's and 1980's also natural sciences notably mineralogy and vegetation science started systematically to measure optical properties of leaves and minerals/rocks with spectrometers. In the last decade spectroscopy has made the step from qualitative observations of mineral classes, soil type and vegetation biomass to quantitative estimates of mineral, soil and vegetation chemistry. This resulted in geothermometers used to characterize metamorphic and hydrothermal systems and to the advent of foliar biochemistry. More research is still needed to bridge the gap between laboratory spectroscopy and field spectroscopy. Empirical studies of minerals either as soil or rock constituents (and vegetation parameters) derived from regression analysis of spectra against chemistry is important in understanding the physics of the interaction of electromagnetic radiation and matter which in turn is important in the design of future satellite missions. Physics based models and retrievals are needed to operationalize these relationships and implement them in future earth observation missions as these are more robust and easy to transfer to other areas and data sets.

1. Introduction

Spectroscopy is the science concerned with the investigation and measurement of spectra produced when materials interact with or emits electromagnetic radiation. These spectra have been used to chemically characterize earth science materials and to classify them based on diagnostic absorption features that result from molecular vibrational and electronic processes of water molecules, OH groups and other bonds. Over the last decade we have seen many studies that attempt to quantify chemical constituents in water, vegetation, soil, minerals and rocks. Most of these studies use empirical models while some try to develop full inversions based on physical radiative transfer models.

The history of spectrometric measurements dates back to the early 1900's. In 1913, Twyman (part of the Hilger company, UK) designed the first infrared spectrometer. In 1933 and 1944 respectively Kipp and sons in out of the Netherlands and Grubb and Parsons manufactured infrared spectrometers. After world war 2, both US-based Beckman and Perkin-Elmer started the commercial production of infrared spectrometers. However the history of infrared spectrometry dates back to 1823 when Fraunhofer invented the grating which made light dispersion into wavelengths possible (Fraunhofer, 1823). A review of early methods and instrumentation for infrared spectrometry is found in a

paper by Bowling Barnes and Bonner (Bowling Barnes and Bonner, 1936).

In the 1950's–1970's researcher were looking at unravelling optical properties of plants (Billings and Morris, 1951; Gates et al., 1965; McClellan et al., 1963). In the 1970's, Graham Hunt and John Salisbury (later joined by Charles Lenhoff) systematically measured spectra of minerals and later rocks and analyzed these spectra linking the diagnostic absorption found to the mineral chemistry and structure. As such their studies resulted in the first spectral libraries of minerals and their interpretation proved to be the 'Rosetta stone' for modern geological remote sensing; allowing scientists to unravel the complex signal of early imaging systems. They started working on silicate minerals (Hunt and Salisbury, 1970) and continued working on carbonates (Hunt and Salisbury, 1971), oxide minerals (Hunt et al., 1971a), sulphide minerals (Hunt et al., 1971b), and salts (Hunt et al., 1972). Next they analyzed rocks starting with igneous rocks (Hunt et al., 1973a,b, 1974), sedimentary rocks (Hunt and Salisbury, 1976a), and metamorphic rocks (Hunt and Salisbury, 1976b).

The United States Department of Agriculture in the 1970's through 1980's (Dixit and Ram, 1985; Norris et al., 1976) performed systematic spectral measurements of dried and ground leaves and related absorption features to foliar chemistry. Probably the first to make the link

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between foliar chemistry and potential for remote sensing were Carol Wessman (Wessman et al., 1988a, 1988b) and Paul Curran (Curran, 1989). These early review papers mark the onset of foliar chemistry using the relationship of particular plant compounds to absorption features. Why do foliar chemistry and try to quantify plant compounds? Chlorophyll is an indicator of plant productivity, nitrogen is a proxy for the availability of nutrients, lignin level is correlated with plant (cellulose) decomposition and the vegetation spectral red-edge is a measure of plant health (stress). These are observations that are relevant for agriculture crop monitoring and yield prediction, for understanding ecosystem functioning, understanding the carbon cycle and the carbon exchange between vegetation and the atmosphere in global change studies. What plant compounds are spectrally active? Biochemical constituents of leaves that can be studied spectroscopically are cellulose, lignin, starch and (nitrogen-based) components such as proteins and chlorophyll. More particularly, in the visible part of the spectrum pigments such as chlorophyll a and b, carotene and xanthophyll determine the reflective properties of leaves. An overview of regression based methods for foliar chemistry is found in (Kokaly and Clark, 1999). There is a wealth of papers showing the potential of quantifying leaf chlorophyll content for various crops and vegetation species (Daughtry et al., 2000; Gitelson and Merzlyak, 1997). The foliar biochemistry community made the step from leaf to canopy estimation thus addressing scale issues and also made the step from empirical to physical models thus allowing transferability and repeatability of retrievals. Hence it serves as a good example for directions the soil and geology communities working on spectroscopy could take.

The last 10 years or so have seen many applications of spectroscopy to quantify the chemical composition of minerals and rocks. In this paper an overview is provided of recent (< 10 year old) studies on quantitative spectroscopy to estimate mineral (soil, rock) chemistry. This paper brings together some of that work (with no intention to provide an all-inclusive overview) closely linking spectroscopy to analytical chemistry with an outlook to the potential for global earth observation and monitoring of earth system variables.

2. Some theoretical considerations

2.1. Background

Electromagnetic radiation is a wave motion which is a stream of particles or a stream of photons. Therefore a common measurement unit of radiation is the wavenumber or the number of waves per cm. The spectroscopic wavenumber is the reciprocal of the wavelength of light in a vacuum. Vice versa many spectrometers use micrometer or nanometer as the unit of measurement. Reflectance is a function of scattered radiance from the surface and the incident irradiance intensity. Usually reflectance is measured by the ratio of the intensity reflected from a sample divided by that of a standard or reference. Commonly used measurement principles are hemispherical-conical (also referred to as hemispherical-directional) reflectance and biconical reflectance (Milton et al., 2009).

2.2. Instrument characteristics

The following are key characteristics for spectrometers from a user perspective: (1) spectral range, (2) spectral bandwidth, (3) spectral sampling interval, and (4) signal-to-noise ratio (SNR).

The spectral ranges (and definitions) that are commonly used in spectrometry include the: visible (VIS: 0.4–0.7 μm), near-infrared (NIR 0.7–1.4 μm), short-wave infrared (SWIR: 1.4–3 μm), mid-infrared (MIR: 3–8 μm), longwave infrared (LWIR) or thermal infrared (TIR: 8–15 μm). It should be noted that this division is dependent on the discipline and application. For example, the International Commission on Illumination, the ISO 20473 scheme and the field of astronomy use slightly different definitions. The manufacturers of spectrometers

typically coin the different wavelength regions to the type of detectors and their sensibility. The near-infrared is linked to the sensitivity of silicon (0.7–1.0 μm), the short-wave infrared to InGaAs (1.0–3 μm), the mid-infrared (3–5 μm) to Indium Antimonide and HgCdTe and the Long-wave infrared (7–14 μm) to HgCdTe and microbolometers.

Spectral bandwidth is loosely defined as the width of an individual spectral channel in a spectrometer. This is important as it determines the width of a diagnostic absorption feature that can be resolved by the spectrometer. Spectral sampling interval is the distance in wavelength between adjacent spectral bands (or band passes or channels or spectral response functions of channels) in a spectrometer.

Spectral resolution in remote sensing is a measure of the ability of a sensor to capture fine wavelength intervals and this often is the product of spectral sampling and spectral bandwidth. The International Union of Pure and Applied Chemistry defines spectral resolution in optical spectroscopy as “the minimum wavenumber, wavelength or frequency difference between two lines in a spectrum that can be distinguished”.

The signal-to-noise ratio is more subjective. By definition noise is random variability of the signal and signal is the quantity of light measured by the spectrometer. Two prevailing methods are typically used to quantify the signal-to-noise ratio of a spectrometer: one based on laboratory calibration measures and the second using instrument measures. Signal mean over signal standard deviation is a typical laboratory based measurement. Often reference targets are used for this. Using the instrument dark current (shutter closed) of the spectrometer is an often used instrument method. Manufacturers often also report the so-called Noise Equivalent Spectral Radiance (NESR). This NESR is the spectral radiance required to obtain a SNR of 1.

2.3. Field spectrometers

The reader is also referred to a review paper by Milton et al. who summarized measurement geometries, give an overview of available instruments back in 2009, review principles of multiple view angle acquisitions, and give examples of field spectroscopy for vicarious calibration and atmospheric corrections (Milton et al., 2009).

The Geophysical Environmental Research Corporation (GER) was one of the early manufacturers of near infrared spectrometers. More recently, with the technology developed at GER, SPECTRAL EVOLUTION (<http://www.spectralevolution.com/>) markets state of the art UV–vis–NIR–SWIR full range spectroradiometers for use in the field and in the laboratory. Likewise since 1990, Analytical Spectral Devices (ASD) built spectrometers and still is manufacturing spectroradiometers (<https://www.asdi.com/>). One of the early (and now out of production) systems is the so-called portable infrared mineral analyzer (PIMA) developed by the Australian Integrated Spectronics Pty Ltd. With a built in light source this instrument senses the SWIR and is customized for mineralogical studies. Within the LWIR/TIR (typically starting from the SWIR) Fourier transform infrared spectroscopy (FTIR) is used which is a technique to obtain an infrared spectrum of absorption and emission. These FTIR instruments are typically designed for solids (quality control pharmaceutical applications), liquids and gases, but there are several custom designs for studying rocks and (to a lesser extent) vegetation. Companies that manufacture such instruments include Bruker (<http://www.bruker.com>), Thermofisher (<https://www.thermofisher.com/>) which markets the Nicolet series FTIR systems and the MIDAC corporation (<http://midac.com/>). Finnish company SPECIM (<http://www.specim.fi/>) designs hyperspectral imaging camera systems for use in the laboratory and field.

Over the years several spectral libraries have been compiled following the pioneering work of Graham Hunt and John Salisbury who measured and collected spectra of many mineral and rock groups. To highlight a view: the NASA Jet propulsion laboratory of 160 minerals (https://speclib.jpl.nasa.gov/documents/jpl_desc), the USGS spectral library (<https://speclab.cr.usgs.gov/spectral-lib.html>), the John Hopkins University spectral library (Salisbury et al., 1991) of Salisbury

(https://speclib.jpl.nasa.gov/documents/jhu_desc) and the ASTER spectral library (<https://speclib.jpl.nasa.gov/>) which combines parts of the JHU, JPL and USGS spectral libraries documenting over 2400 spectra of natural and man-made materials (Baldrige et al., 2009). Most of these libraries contain spectra of geologic materials (minerals and rocks) and to a lesser extent and also less well-structured information about vegetation spectral properties at species level (and in some cases man-made materials). It is worthwhile to mention a number of global (Rossel et al., 2016; Shepherd and Walsh, 2002) and regional initiatives (Brodsky et al., 2011) to come to soil spectral databases, however although there is a standard nomenclature for soils, these libraries are typically area specific.

2.4. Spectral transformation techniques

The wavelength position of an absorption feature can be typically linked to the chemistry of a substance while the depth of the absorption feature is proportional to the abundance of a substance. For minerals, subtle shifts of the position of an absorption feature can be correlated to subtle differences in chemistry as for example Al-Mg compositional changes in white micas (Duke, 1994) and Ca-Mg compositional changes in limestones (Gaffey, 1986). To make full use of empirical methods to predict mineral chemistry from spectral information some standardization of spectra is often needed. A regularly used transformation technique is the so-called continuum removal (Clark and Roush, 1984). The continuum of a spectrum is the background reflectance or the overall concave shape of the spectral curve. By fitting a continuum, kind of a rubber band over the spectrum, and removing the background spectral signal the individual absorption features are singled out and the spectral curve is standardized where no absorption is 100%. Modern versions of the Hull removal technique rather than fitting one curve over the spectrum fit many local Hull straight-line curves over the spectrum as these are less influenced by grain size effects and illumination difference effects (Clark et al., 2003). For more details and a review of spectral processing methods for geological remote sensing the reader is referred to (Asadzadeh and de Souza, 2016).

3. Empirical studies

In this section, studies relating near infrared spectroscopy to chemistry of minerals in the context of whole rock geochemistry and soil mineralogy are presented and reviewed.

3.1. Geology and minerals

Some of the early studies looking into mineral chemistry predicted from near infrared spectra focused on unravelling regional metamorphic grade. In particular the Al-O-H absorption band in muscovite shows a systematic shift from 2217 nm to 2199 nm in the biotite zone which allows to map regional metamorphic facies (Duke, 1994; Duke and Lewis, 2010). Similarly it was shown that quantitative analysis of SWIR spectra enabled to classify rock samples into the metamorphic amphibolite and greenschist facies (Abweny et al., 2016).

Abundance estimates of muscovite (white mica) in particular mapping the change in Al content which is reflected in a shift in the Al-OH absorption feature in altered volcanic rock vary systematically along fossil fluid pathways (Van Ruitenbeek et al., 2005). This allowed to use Al-OH to Mg-OH variations to be used to map zones of low-temperature recharge gradually up to zones of high-temperature discharge. Thus spectroscopy has been shown to be able to map hydrothermal fluid chemistry, temperature of alteration, coexisting minerals, and composition of volcanic host rock (Van Ruitenbeek et al., 2006).

There are several studies looking at spectroscopy as a tool to estimate and map mining pollution. A classic study focused on the Aznacollar spill in Spain (Kemper and Sommer, 2002) looking at the dispersion of various heavy metals. A related study focused on soil

pollution in a Polish mine site (Siebielec et al., 2004) and another example is a study on Cu-Zn mine waste monitoring in the Penn mine in Sierra Nevada, California (Montero et al., 2005).

Using TIR/LWIR spectroscopy, feldspars were studied. FTIR spectra were shown to be able to map K-, Na- and Ca- feldspar concentrations (Matteson and Herron, 1993). More recently, partial least squares regression models were developed to link the thermal infrared spectra to the thin section determined mineral modes of alkali feldspar through to the plagioclase endmember (Hecker et al., 2010).

A number of studies focused on carbonate spectroscopy with the common notion that the carbonate absorption feature in the 2.3–2.35 mm range shifts with the Ca-Mg ratio of the sample thus enabling to quantify the amount of dolomite versus calcite in a sample (Gaffey, 1986; Van der Meer, 1995). It has been shown that SWIR spectra can be used to predict the calcite/dolomite ratio of a rock sample (Zaini et al., 2014) which is relevant when studying oil and gas reservoirs as dolomite is more porous than calcite and thus can host more oil.

3.2. Soil properties

There are several motivations to study soils using near infrared spectroscopy and attempting to arrive at unified relationships in support of remote sensing studies. Soil parameters are important input to erosion and land degradation models (de Jong et al., 1999; Shrestha et al., 2005), several soil parameters directly link to soil fertility which is important in agronomy and agriculture (Vagen et al., 2006), various human activities result in soil pollution which needs to be contained or soils need to be cleaned up (Kopackova et al., 2012) and soil are usually the substrate for manmade constructions hence understanding engineering properties of soils is important (Jones and Holtz, 1973).

Early studies used multiple linear regression analysis to predict soil properties from spectra, which can be used to model relationships between a small number of predictors and response variables, because with an increase in number of predictors it will not perform well due to multicollinearity problems (Wold et al., 1984). Therefore most soil studies started using partial least squares regression (PLSR) analysis; a technique that stems from the chemometrics field and has been used for routine quality control activities in the chemical, the pharmaceutical and agro-industries.

PLSR was developed by Herman Wold (Wold et al., 2001) as a regression by means of projections to latent variables. It typically uses a set of predictors (typically near infrared reflectance spectra) and a set of dependent response variables (the soil properties of interest).

Root mean square error of calibration (RMSEC) and prediction (RMSEP) are used to drive the model and measure the difference between the predicted and measured response values at the calibration and validation stages. Further the so-called interference error or bias, which is the systematic error due to the un-modelled variables in the spectral data is used in an iteratively minimization process. PLSR is particularly well-suited when dealing with a large number of (predictor, response) variables when multicollinearity issues are lurking.

3.2.1. Soil parameter quantification

Soil spectroscopy started to gain attention with the work of Stoner and co-authors in the 1970's and early 1980's (Stoner et al., 1980). Since then many studies have shown the potential of using near-infrared spectra to quantify a multitude of soil parameters. A classic paper used partial least-squares regression to model soil properties including pH, organic carbon, texture, cation exchange capacity, phosphorus and electrical conductivity (Rossel et al., 2006). Another early paper advocated the use of spectra to replace soil chemical analysis thus starting a new field of science namely soil spectroscopy (Bendor and Banin, 1995). Partial least squares regression using spectra of soils against a soil property database proved that rapid chemometric techniques are suited for simultaneous analysis of soil properties (Janik and Skjemstad,

1995; Nocita et al., 2015). Most studies focus on the near-infrared and shortwave infrared spectral region as these show the most diagnostic absorption features that can be correlated to soil chemistry. Recently some studies have shown there is merit in studying the longwave or thermal infrared region (Choe et al., 2010; Eisele et al., 2012; Sobrino et al., 2009) to quantify soil parameters as this provides synergistic information compared to the SWIR region.

Several studies focused on quantifying soil organic carbon as this is an important parameter that relates to the nutrition of soils (Bartholomeus et al., 2008; Stevens et al., 2008; Vasques et al., 2009). In addition, salinity issues have also been addressed using spectroscopy as soil salinization deteriorates the use of soil as a resource for agriculture (Aldabaa et al., 2015; Farifteh et al., 2007; Farifteh et al., 2008). Other related studies focused on soil nitrates which are important in terms of soil fertilization (Choe et al., 2010; Linker, 2004).

To describe and classify soils, traditional soil science amongst others looks at soil color. This is done in the field using the Munsell color chart. Several papers have proposed to use soil spectra and turn the RGB measured reflectance into a quantitative estimate of soil color (Galvao et al., 1997; Mouazen et al., 2007).

Soil moisture is a disturbing factor in soil spectral analysis. In many studies this has either been discarded or by-passed by drying the soil prior to spectral analysis. Few studies tried to do spectral retrievals and modeling in the presence of soil moisture (Minasny et al., 2011). There are a number of attempts to estimate soil crusting but it is found that it is rather cumbersome to do that in a reproducible and transferable way (Ben-Dor et al., 2003; Dejong, 1992; Goldshleger et al., 2002). Lastly it should be mentioned that some paper have appeared looking into soil aggregate stability (Gomez et al., 2013; Ymeti et al., 2017).

3.2.2. Soil contamination

Several researchers that studied the use of soil near infrared spectra to quantify soil contamination and pollution. A number of papers focused on heavy metals such as cadmium and zinc (Kooistra et al., 2001), arsenic (Ren et al., 2009) and mercury (Wu et al., 2005b) both in floodplains as well as in-situ in soils. One of the common misconceptions in such research is that the spectra through a PLSR correlation analysis are predicting the spectral responses of the heavy metals. However these are spectrally featureless, so the measured response is an indirect response typically related to the soil composition as the heavy metals tend to bind to soil constituents. In addition, there are several studies that looked at soil contamination in relation to mining operations. Choe et al. took a regional perspective looking at dispersion of heavy metals from past mining operations and waste dump sites in gold and copper exploration (Choe et al., 2008), while a study in the Czech republic focused on mapping of soil Ph in a coal mining area (Kopackova, 2014). Current research also focuses on cleaning – up technologies for heavy metal polluted areas (often former mining areas). Phytoremediation is one such new and promising technologies that uses plants to remove toxic contaminants from heavy metal polluted soils (Hassan et al., 2008; Rathod et al., 2013).

3.2.3. Soil engineering

Other soil properties that have been studied using near infrared spectroscopic measurements relate to engineering parameters of soil strength. There are several standard geoenvironmental tests that are in use to determine the soil strength such as the liquid limit test, plastic limit test, plasticity index and the more general coefficient of linear extensibility (COLE) and cation exchange capacity (CEC). Expansive soils easily swell and shrink causing structural damage to buildings and other infrastructure (Jones and Holtz, 1973). Typically soil expansiveness is related to the amount of organic carbon in the soil on the one hand and the mineralogy of the soil on the other hand. The swelling potential of a soil depends largely on the clay mineralogy of the soil where the two layer kaolinites exhibit low swell while the three layer smectites (and to a lesser extent illites) exhibit high swelling potential

as they can store water between the layers and thus swell and shrink with changes in water availability. Several studies have focused on spectrally mapping the clay mineralogy of soils as a proxy to swelling potential mostly using the SWIR spectral region (Chabrilat et al., 2002; Goetz et al., 2001; Kariuki and van der Meer, 2004; Ulusoy et al., 2016; Waruru et al., 2014; Yitagesu et al., 2009) but also some exploiting the TIR region (Yitagesu et al., 2011).

3.3. Quality control

It is clear from this review that the use of spectral techniques has advanced our understanding of soil and whole rock chemistry which in turn allows us to better predict alteration stages, grade of metamorphism and soil engineering properties. Geologists have also started to use spectroscopy as a means of quality control. In fact, spectroscopy is an accepted method for quality control in the pharmaceutical industry (Reich, 2005; Roggo et al., 2007) and in various sectors of the food industry (Huang et al., 2008). In mining spectral measurements have been used (in the laboratory and also in the field) to estimate ore grades. For example in iron ore deposits a study has been looking at the goethite-hematite ratio which is a proxy for aluminum, phosphorus and silica (Cudahy and Ramanaidou, 1997). Another research line focuses on reducing the amount of mining waste by improving the efficiency of the production process through better quantifying of the mineralogy of ore samples. Traditionally this is done through x-ray diffraction and x-ray fluorescence combined with atomic absorption spectroscopy (Tathavadkar et al., 2004). A good review and early study showed the potential of spectroscopy on conveyor belts for ore to waste separation (Goetz et al., 2009). More recently, studies commenced looking at real-time ore sorting using spectral measurements on porphyry copper to distinguish copper grades (Dalm et al., 2017; Dalm et al., 2014; Iyakwari and Glass, 2014). Another example of quality control is using the carbonate absorption feature to quantify the amount of dolomite in limestones as a proxy to rock quality for making cement (Zaini et al., 2016).

3.4. Scaling issues

Issues of scale in remote sensing (Moody and Woodcock, 1995; Woodcock and Strahler, 1987), upscaling and downscaling of parameters have been researched since the advent of earth observation satellites. These are also relevant to spectral measurements as these are done at different scales: contact spot measurements, measurements with a spectrometer on a tripod of surfaces from a distance in the order of a meter or less, measurements with a spectrometer in a cherry picker at several meters height. A special issue on this topic brought together some classic papers (Quattrochi and Atkinson, 1999) and also a book was published on this topic (Quattrochi and Goodchild, 1997). More recently, a paper reviewed scale issues in remote sensing providing a good reference basis for the definition of various meanings of scale in a spatial and geographic context as well as providing an overview of methods for scaling of measurements, retrievals and remote sensing products (Wu and Li, 2009). There are few studies actually addressing and modeling change of remote sensing signal and products over different scales. Approaches that have been proposed either try to do this through physical models (Raffy, 1992) or by using concepts arising from geostatistics and spatial statistics (see for a review (Van der Meer, 2012)).

The vegetation community worked on the scaling of biochemical parameters from single leaf to canopy level. A classic paper addressing the scaling from leaf to canopy is (Asner and Martin, 2008) and a good review of the field is provided by (Majeke et al., 2008). There are several papers showing the estimation of leaf nitrogen using spectroscopic measurements at leaf and canopy scale and various crops (Johnson and Billow, 1996; Kokaly, 2001; Ramoelo et al., 2013; Yoder and Pettigrewcrosby, 1995) and several papers focusing on lignin

(Brinkmann et al., 2002; Hodge and Woodbridge, 2004) and cellulose (McLellan et al., 1991; Wu et al., 2005a). It has also been demonstrated that similar foliar biochemical retrievals can be done spatially using airborne hyperspectral sensors such as AVIRIS (Asner et al., 2011; Gao and Goetz, 1995; Kokaly et al., 2003; Serrano et al., 2002), HyMAP (Huang et al., 2004; Mutanga et al., 2005) and, for example, CASI data (Croft et al., 2013). This forms the basis of concepts such as the global biodiversity essential variables (Chandler et al., 2017; Pereira et al., 2013; Pettorelli et al., 2016; Proenca et al., 2017) and mission concepts for HypSIRI NASA's Hyperspectral Infrared Imager (Lee et al., 2015) and the German EnMAP system (Guanter et al., 2015).

The geology and mineralogy community has only recently started looking into scaling issues in relation to spectral measurements. This is driven by the advent of laboratory-based imaging spectrometers that allow imaging of rock samples (Baissa et al., 2011), thin sections and drill core (Schodlok et al., 2016; Tappert et al., 2011). This allows to look at the estimation of bulk mineralogy of rock samples at different scales such as scales representative of a thin section, or a hand specimen or rock sample, or a cored rock of different lengths or an outcrop. Typically laboratory based imaging spectrometers allow to measure at different spatial resolutions varying from around 20 micrometer up to 400 mm. This poses interesting issues related to scale as at the high resolution each pixel is nearly composed of one mineral while at the lower resolution a pixel is a mixture of minerals.

Similarly mine face scanning with imaging spectrometers has been done to bridge the gap between field and airborne/satellite observations in the realm of geology (Buckley et al., 2013; Kurz and Buckley, 2016).

4. Discussion

In this paper it has been shown that over the last decade spectroscopy has made the step from qualitative observations of mineral classes, soil type and vegetation biomass to quantitative estimates of mineral, soil and vegetation chemistry. In geology this has resulted in geothermometers based on spectral absorption properties of minerals (Duke, 1994), in soil science we have seen the first continent-wide seamless map products (Cudahy et al., 2010; Hewson et al., 2005), and foliar chemistry allows the retrieval of essential vegetation variables (Pereira et al., 2013). More research is still needed to bridge the gap between laboratory spectroscopy and field spectroscopy (Johnson et al., 1998).

Empirical studies of mineral, soil, and vegetation parameters derived from regression analysis of spectra against chemistry is important in understanding the physics of the interaction of electromagnetic radiation and matter which in turn is important in the design of future satellite missions. For example, ESA's medium-spectral resolution imaging spectrometer (MERIS) had dedicated narrow spectral bands for chlorophyll measurements (Rast et al., 1999). In the near future we see the German EnMAP hyperspectral mission (Stuffer et al., 2007) being launched and empirical studies allow us to better make use of EnMAP data and in a more distant future of data from the NASA's Hyperspectral Infrared Imager (HypSIRI) mission (Lee et al., 2015). FLEX, the Fluorescence Explorer mission (Stoll et al., 2003), is one of ESA's earth explorer missions that aims to map vegetation fluorescence as a proxy to photosynthetic activity using the 0.5–0.8 μm region. This provides a handle on carbon exchange between vegetation and the atmosphere and provides insights into how carbon and water cycles are influenced by photosynthesis. The spectral bandwidth is in the order of 0.3 nm (with a spectral sampling interval of 0.1 nm), thus very targeted observations. Empirical spectroscopic studies are essential in ensuring proper band positioning of such high resolution imagers.

Empirical studies are good to understand relationships between spectroscopy of earth materials and their chemistry. However empirical models based on statistics are often poorly transferable to other areas, data sets, sensors, and are not always reproducible. Physics based

models and retrievals are needed to operationalize these relationships and implement them in future earth observation missions. Examples from the vegetation community are the SAIL model (Verhoef, 1984) and the PROSPECT model (Jacquemoud and Baret, 1990) that allow to model reflectance at leaf and canopy level, however for soil and mineral observations no such models exist. However, recently we have seen several studies where outcrops are imaged with high spectral resolution imaging spectrometers (Bellian et al., 2007; Kurz et al., 2013), which offers good prospect to bridge the scale difference between the laboratory and the field and it in potential also allows to arrive at scalable products to be linked to airborne and spaceborne remote sensing observations. In geology there are a number of algorithms that have been developed that try to use absorption feature position and wavelength as a proxy to mineral chemistry. The USGS Tetracorder algorithm was one of the early absorption feature fitting expert-based systems (Clark et al., 2003). More recently, the remote sensing team at the Czech geological survey published the so-called 'quantools' algorithm (Kopackova and Koucká, 2017) and at ITC the 'wavelength mapper' algorithm was published (Bakker et al., 2011; van Ruitenbeek et al., 2014). These algorithms automatically extract the wavelength position and depth of various mineral absorption features which can be linked to subtle differences in mineral chemistry (Van der Meer et al., 2018).

The advent of laboratory and field based hyperspectral imaging cameras allows the geology community to start addressing the issue of scale in spectroscopy and spectral measurements. Hand specimen can be measured at different spatial scales to understand the effect of mineral mixing on the spectral response and how this in turn affects the quantification of mineralogical composition of a sample. In addition, large surfaces can be imaged in the field (Kurz et al., 2013) with these instruments which allows detailed characterization of CalVal targets.

5. Conclusions

There is an active community of scientists studying the empirical relationships between reflectance (and emittance) spectra and the chemistry of minerals, soils and vegetation using laboratory spectroscopic measurements. This has resulted in a better understanding of the key absorption features and their relationship to essential climate, biodiversity and soil parameters and this has led to proxies for geothermometers in geology. These empirical relationships are essential to programming future satellite missions and enable the community to make better use of present high spectral resolution airborne and spaceborne sensors. There is still a need to further explore the stability of such empirical relationships under field conditions and to address issues related to scaling, transferability and reproducibility of models in space and time.

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References

- Abweny, M.S., van Ruitenbeek, F.J.A., de Smeth, B., Woldai, T., van der Meer, F.D., Cudahy, T., Zegers, T., Blom, J.K., Thuss, B., 2016. Short-wavelength Infrared (SWIR) spectroscopy of low-grade metamorphic volcanic rocks of the Pilbara Craton. *J. Afr. Earth. Sci.* 117, 124–134.

- Aldabaa, A.A.A., Weindorf, D.C., Chakraborty, S., Sharma, A., Li, B., 2015. Combination of proximal and remote sensing methods for rapid soil salinity quantification. *Geoderma* 239, 34–46.
- Asadzadeh, S., de Souza, C.R., 2016. A review on spectral processing methods for geological remote sensing. *Int. J. Appl. Earth Obs. Geoinf.* 47, 69–90.
- Asner, G.P., Martin, R.E., 2008. Spectral and chemical analysis of tropical forests: scaling from leaf to canopy levels. *Remote Sens. Environ.* 112 (10), 3958–3970.
- Asner, G.P., Martin, R.E., Knapp, Tupayachi, R., Anderson, C., Carranza, L., Martinez, P., Houcheime, M., Sinca, F., Weiss, P., 2011. Spectroscopy of canopy chemicals in humid tropical forests. *Remote Sens. Environ.* 115 (12), 3587–3598.
- Baissa, R., Labbassi, K., Launeau, P., Gaudin, A., Ouajhain, B., 2011. Using HySpex SWIR-320 m hyperspectral data for the identification and mapping of minerals in hand specimens of carbonate rocks from the Ankloute Formation (Agadir Basin Western Morocco). *J. Afr. Earth Sci.* 61 (1), 1–9.
- Bakker, W.H., van Ruitenbeek, F.J.A., van der Werff, H.M.A., 2011. Hyperspectral image mapping by automatic color coding of absorption features. In: 7th EARSEL Workshop of the Special Interest Group in Imaging Spectroscopy. Edinburgh, UK, EARSEL. pp. 56–57.
- Baldrige, A.M., Hook, S.J., Grove, C.I., Rivera, G., 2009. The ASTER spectral library version 2.0. *Remote Sens. Environ.* 113 (4), 711–715.
- Bartholomeus, H.M., Schaepman, M.E., Kooistra, L., Stevens, A., Hoogmoed, W.B., Spaargaren, O.S.P., 2008. Spectral reflectance based indices for soil organic carbon quantification. *Geoderma* 2, 28–36.
- Bellian, J.A., Beck, R., Kerans, C., 2007. Analysis of hyperspectral and lidar data: remote optical mineralogy and fracture identification. *Geosphere* 3 (6), 491–500.
- Ben-Dor, E., Goldshleger, N., Benyamini, Y., Agassi, M., Blumberg, D.G., 2003. The spectral reflectance properties of soil structural crusts in the 1.2- to 2.5- μ m spectral region. *Soil Sci. Soc. Am. J.* 67 (1), 289–299.
- Bendor, E., Banin, A., 1995. Near-infrared analysis (NIRA) as a method to simultaneously evaluate spectral featureless constituents in soils. *Soil Sci.* 159 (4), 259–270.
- Billings, W.D., Morris, R.J., 1951. Reflection of visible and infrared radiation from leaves of different ecological groups. *Am. J. Bot.* 38 (5), 327–331.
- Bowling Barnes, R., Bonner, L.G., 1936. The early history and the methods of infrared spectroscopy. *Am. Phys. Teacher* 1, 181–189.
- Brinkmann, K., Blaschke, L., Polle, A., 2002. Comparison of different methods for lignin determination as a basis for calibration of near-infrared reflectance spectroscopy and implications of lignoproteins. *J. Chem. Ecol.* 28 (12), 2483–2501.
- Brodsky, L., Klement, A., Penizek, V., Kodesova, R., Boruvka, L., 2011. Building soil spectral library of the Czech soils for quantitative digital soil mapping. *Soil Water Res.* 6 (4), 165–172.
- Buckley, S.J., Kurz, T.H., Howell, J.A., Schneider, D., 2013. Terrestrial lidar and hyperspectral data fusion products for geological outcrop analysis. *Comput. Geosci.* 54, 249–258.
- Chabrilat, S., Goetz, A.F.H., Krosley, L., Olsen, H.W., 2002. Use of hyperspectral images in the identification and mapping of expansive clay soils and the role of spatial resolution. *Remote Sens. Environ.* 82 (2–3), 431–445.
- Chandler, M., See, L., Copas, K., Bonde, A.M.Z., Lopez, B.C., Danielsen, F., Legind, J.K., Masinde, S., Miller-Rushing, A.J., Newman, G., Rosemartin, A., Turak, E., 2017. Contribution of citizen science towards international biodiversity monitoring. *Biol. Conserv.* 213, 280–294.
- Choe, E., van der Meer, F., Rossiter, D., van der Salm, C., Kim, K.W., 2010. An alternate method for Fourier transform infrared (FTIR) spectroscopic determination of soil nitrate using derivative analysis and sample treatments. *Water Air Soil Pollut.* 206 (1–4), 129–137.
- Choe, E., van der Meer, F., van Ruitenbeek, F., van der Werff, H., de Smeth, B., Kim, Y.W., 2008. Mapping of heavy metal pollution in stream sediments using combined geochemistry, field spectroscopy, and hyperspectral remote sensing: a case study of the Rodalquilar mining area. SE Spain: *Remote Sens. Environ.* 112 (7), 3222–3233.
- Clark, R.N., Roush, T.L., 1984. Reflectance spectroscopy – quantitative-analysis techniques for remote-sensing applications. *J. Geophys. Res.* 89 (NB7), 6329–6340.
- Clark, R.N., Swayze, G.A., Livo, K.E., Kokaly, R.F., Sutley, S.J., Dalton, J.B., McDougall, R.R., Gent, C.A., 2003. Imaging spectroscopy: earth and planetary remote sensing with the USGS Tetracorder and expert systems. *J. Geophys. Res.-Planets* 108, E12.
- Croft, H., Chen, J.M., Zhang, Y., Simic, A., 2013. Modelling leaf chlorophyll content in broadleaf and needle leaf canopies from ground, CASI, Landsat TM 5 and MERIS reflectance data. *Remote Sens. Environ.* 133, 128–140.
- Cudahy, T.J., Caccetta, M., Chia, J., Collings, S., Hewson, R.D., 2010. Towards global mapping of the earth's land surface composition. In: In: Kajiwar, K., Muramatsu, K., Soyama, N., Endo, T., Ono, A., Akatsuka, S. (Eds.), *Networking the World with Remote Sensing* 38. pp. 459–463.
- Cudahy, T.J., Ramanaidou, E.R., 1997. Measurement of the hematite:goethite ratio using field visible and near-infrared reflectance spectrometry in channel iron deposits, western Australia. *Aust. J. Earth Sci.* 44 (4), 411–420.
- Curran, P.J., 1989. Remote-sensing of foliar chemistry. *Remote Sens. Environ.* 30 (3), 271–278.
- Dalm, M., Buxton, M.W.N., van Ruitenbeek, F.A., 2017. Discriminating ore and waste in a porphyry copper deposit using short-wavelength infrared (SWIR) hyperspectral imagery. *Miner. Eng.* 105, 10–18.
- Dalm, M., Buxton, M.W.N., van Ruitenbeek, F.J.A., Voncken, J.H.L., 2014. Application of near-infrared spectroscopy to sensor based sorting of a porphyry copper ore. *Miner. Eng.* 58, 7–16.
- Daughtry, C.S.T., Walthall, C.L., Kim, M.S., de Colstoun, E.B., McMurtrey, J.E., 2000. Estimating corn leaf chlorophyll concentration from leaf and canopy reflectance. *Remote Sens. Environ.* 74 (2), 229–239.
- de Jong, S.M., Paracchini, M.L., Bertolo, F., Folving, S., Megier, J., de Roo, A.P.J., 1999. Regional assessment of soil erosion using the distributed model SEMMED and remotely sensed data. *Catena* 4, 291–308.
- Dejong, S.M., 1992. The analysis of spectroscopical data to map soil types and soil crusts of Mediterranean eroded soils. *Soil Technology* 5 (3), 199–211.
- Dixit, L., Ram, S., 1985. Quantitative-analysis by derivative electronic spectroscopy. *Appl. Spectrosc. Rev.* 21 (4), 311–418.
- Duke, E.F., 1994. Near-infrared spectra of muscovite, Tschermark substitution and metamorphic reaction process – implications for remote sensing. *Geology* 22 (7), 621–624.
- Duke, E.F., Lewis, R.S., 2010. Near infrared spectra of white mica in the Belt Supergroup and implications for metamorphism. *Am. Mineral.* 95 (7), 908–920.
- Eisele, A., Lau, I., Hewson, R., Carter, D., Wheaton, B., Ong, C., Cudahy, T.J., Chabrilat, S., Kaufmann, H., 2012. Applicability of the thermal infrared spectral region for the prediction of soil properties across semi-arid agricultural landscapes. *Remote Sensing* 4 (11), 3265–3286.
- Farifteh, J., Van Der Meer, F., Carranza, E.J.M., 2007. Similarity measures for spectral discrimination of salt-affected soils. *Int. J. Remote Sens.* 28 (23), 5273–5293.
- Farifteh, J., van der Meer, F., van der Meijde, M., Atzberger, C., 2008. Spectral characteristics of salt-affected soils: a laboratory experiment. *Geoderma* 145 (3–4), 196–206.
- Fraunhofer, J., 1823. Kurzer bericht von den resultaten neuerer versuche uber die gesetze des lichtes und die theorie derselben. *Gilberts Ann.* 74, 337–378.
- Gaffey, S.J., 1986. Spectral reflectance of carbonate minerals in the visible and near-infrared (0.35–2.55 microns) – Calcite, aragonite, and dolomite. *Am. Mineral.* 71, 151–162.
- Galvao, L.S., Vitorello, I., Formaggio, A.R., 1997. Relationships of spectral reflectance and color among surface and subsurface horizons of tropical soil profiles. *Remote Sens. Environ.* 61 (1), 24–33.
- Gao, B.C., Goetz, A.F.H., 1995. Retrieval of equivalent water thickness and information related to biochemical-components of vegetation canopies from AVIRIS data. *Remote Sens. Environ.* 52 (3), 155–162.
- Gates, D.M., Keegan, H.J., Schleter, J.C., Weidner, V.R., 1965. Spectral properties of plants. *Appl. Opt.* 4 (1) 11–8.
- Gitelson, A.A., Merzlyak, M.N., 1997. Remote estimation of chlorophyll content in higher plant leaves. *Int. J. Remote Sens.* 18 (12), 2691–2697.
- Goetz, A.F.H., Chabrilat, S., Lu, Z., 2001. Field reflectance spectrometry for detection of swelling clays at construction sites. *Field Anal. Chem. Technol.* 5 (3), 143–155.
- Goetz, A.F.H., Curtiss, B., Shiley, D.A., 2009. Rapid gangue mineral concentration measurement over conveyors by NIR reflectance spectroscopy. *Miner. Eng.* 22 (5), 490–499.
- Goldshleger, N., Ben-Dor, E., Benyamini, Y., Blumberg, D., Agassi, M., 2002. Spectral properties and hydraulic conductance of soil crusts formed by raindrop impact. *Int. J. Remote Sens.* 23 (19), 3909–3920.
- Gomez, C., Le Bissonnais, Y., Annabi, M., Bahri, H., Raclot, D., 2013. Laboratory Vis-NIR spectroscopy as an alternative method for estimating the soil aggregate stability indexes of Mediterranean soils. *Geoderma* 209, 86–97.
- Guanter, L., Kaufmann, H., Segl, K., Forster, S., Rogass, C., Chabrilat, S., Kuester, T., Hollstein, A., Rossner, G., Chlebek, C., Straif, C., Fischer, S., Schrader, S., Storch, T., Heiden, U., Mueller, A., Bachmann, M., Muhle, H., Muller, R., Habermeyer, M., Ohndorf, A., Hill, J., Buddenbaum, H., Hostert, P., van der Linden, S., Leitao, P.J., Rabe, A., Doerffer, R., Krasemann, H., Xi, H.Y., Mauser, W., Hank, T., Locherer, M., Rast, M., Staenz, K., Sang, B., 2015. The EnMAP spaceborne imaging spectroscopy mission for earth observation. *Remote Sens.* 7 (7), 8830–8857.
- Hassan, M., Sighicelli, M., Lai, A., Colao, F., Ahmed, A.H.H., Fantoni, R., Harith, M.A., 2008. Studying the enhanced phytoremediation of lead contaminated soils via laser induced breakdown spectroscopy. *Spectrochim. Acta Part B-At. Spectrosc.* 63 (10), 1225–1229.
- Hecker, C., van der Meijde, M., van der Meer, F.D., 2010. Thermal infrared spectroscopy on feldspars – successes, limitations and their implications for remote sensing. *Earth Sci. Rev.* 103 (1–2), 60–70.
- Hewson, R.D., Cudahy, T.J., Mizuhiko, S., Ueda, K., Mauger, A.J., 2005. Seamless geological map generation using ASTER in the Broken Hill-Curnamona province of Australia. *Remote Sens. Environ.* 99 (1–2), 159–172.
- Hodge, G.R., Woodbridge, W.C., 2004. Use of near infrared spectroscopy to predict lignin content in tropical and sub-tropical pines. *J. Near Infrared Spectrosc.* 12 (6), 381–390.
- Huang, H.B., Yu, H.Y., Xu, H.R., Ying, Y.B., 2008. Near infrared spectroscopy for on/in-line monitoring of quality in foods and beverages: a review. *J. Food Eng.* 87 (3), 303–313.
- Huang, Z., Turner, B.J., Dury, S.J., Wallis, I.R., Foley, W.J., 2004. Estimating foliage nitrogen concentration from HYMAP data using continuum removal analysis. *Remote Sens. Environ.* 93 (1–2), 18–29.
- Hunt, G.R., Salisbury, J.W., 1970. Visible and near-infrared spectra of minerals and rocks. I. Silicate minerals. *Mod. Geol.* 1, 283–300.
- Hunt, G.R., Salisbury, J.W., 1971. Visible and near-infrared spectra of minerals and rocks. II. Carbonates. *Mod. Geol.* 2, 23–30.
- Hunt, G.R., Salisbury, J.W., 1976a. Visible and near-infrared spectra of minerals and rocks: XI. Sedimentary rocks. *Mod. Geol.* 5, 211–217.
- Hunt, G.R., Salisbury, J.W., 1976b. Visible and near-infrared spectra of minerals and rocks: XII. Metamorphic rocks. *Mod. Geol.* 5, 219–228.
- Hunt, G.R., Salisbury, J.W., Lenhoff, C.J., 1971a. Visible and near-infrared spectra of minerals and rocks III. Oxides and Hydroxides. *Mod. Geol.* 2, 195–205.
- Hunt, G.R., Salisbury, J.W., Lenhoff, C.J., 1971b. Visible and near-infrared spectra of minerals and rocks, IV. Sulphides and sulphates. *Mod. Geol.* 3, 1–14.
- Hunt, G.R., Salisbury, J.W., Lenhoff, C.J., 1972. Visible and near-infrared spectra of minerals and rocks, V. Halides, arsenates, vanadates, and borates. *Mod. Geol.* 3, 121–132.

- Hunt, G.R., Salisbury, J.W., Lenhoff, C.J., 1973a. Visible and near-infrared spectra of minerals and rocks, VII. Acidic igneous rocks. *Mod. Geol.* 4, 217–224.
- Hunt, G.R., Salisbury, J.W., Lenhoff, C.J., 1973b. Visible and near-infrared spectra of minerals and rocks, VIII. Intermediate igneous rocks. *Mod. Geol.* 4, 237–244.
- Hunt, G.R., Salisbury, J.W., Lenhoff, C.J., 1974. Visible and near-infrared spectra of minerals and rocks, IX. Basic and ultrabasic igneous rocks. *Mod. Geol.* 4, 15–22.
- Iyakwari, S., Glass, H.J., 2014. Influence of mineral particle size and choice of suitable parameters for ore sorting using near infrared sensors. *Miner. Eng.* 69, 102–106.
- Jacquemoud, S., Baret, F., 1990. PROSPECT – a model of leaf optical-properties spectra. *Remote Sens. Environ.* 34 (2), 75–91.
- Janik, L.J., Skjemstad, J.O., 1995. Characterization and analysis of soils using midinfrared partial least-squares. 2. Correlations with some laboratory data. *Aust. J. Soil Res.* 33 (4), 637–650.
- Johnson, J.R., Lucey, P.G., Horton, K.A., Winter, E.M., 1998. Infrared measurements of pristine and disturbed soils 1. Spectral contrast differences between field and laboratory data. *Remote Sens. Environ.* 64 (1), 34–46.
- Johnson, L.F., Billow, C.R., 1996. Spectrometric estimation of total nitrogen concentration in Douglas-fir foliage. *Int. J. Remote Sens.* 17 (3), 489–500.
- Jones, D.E., Holtz, W.G., 1973. Expansive soils – hidden disaster. *Civil Eng.* 43 (8), 49–51.
- Kariuki, P.C., van der Meer, F., 2004. A unified swelling potential index for expansive soils. *Eng. Geol.* 2, 1–8.
- Kemper, T., Sommer, S., 2002. Estimate of heavy metal contamination in soils after a mining accident using reflectance spectroscopy. *Environ. Sci. Technol.* 36 (12), 2742–2747.
- Kokaly, R.F., 2001. Investigating a physical basis for spectroscopic estimates of leaf nitrogen concentration. *Remote Sens. Environ.* 75 (2), 153–161.
- Kokaly, R.F., Clark, R.N., 1999. Spectroscopic determination of leaf biochemistry using band-depth analysis of absorption features and stepwise multiple linear regression. *Remote Sens. Environ.* 67 (3), 267–287.
- Kokaly, R.F., Despain, D.G., Clark, R.N., Livo, K.E., 2003. Mapping vegetation in Yellowstone National Park using spectral feature analysis of AVIRIS data. *Remote Sens. Environ.* 84 (3), 437–456.
- Kooistra, L., Wehrens, R., Leuven, R., Buydens, L.M.C., 2001. Possibilities of visible-near-infrared spectroscopy for the assessment of soil contamination in river floodplains. *Anal. Chim. Acta* 446 (1–2), 97–105.
- Kopackova, V., 2014. Using multiple spectral feature analysis for quantitative pH mapping in a mining environment. *Int. J. Appl. Earth Obs. Geoinf.* 28, 28–42.
- Kopackova, V., Chevrel, S., Bourguignon, A., Rojik, P., Ieee, 2012. Mapping hazardous low-PH material in mining environment: multispectral and hyperspectral approaches. 2012 IEEE International Geoscience and Remote Sensing Symposium 2695–2698.
- Kopackova, V., Koucká, L., 2017. Integration of absorption feature information from visible to longwave infrared spectral ranges for mineral mapping. *Remote Sens.* 9 (10), 1006.
- Kurz, T.H., Buckley, S.J., 2016. A review of hyperspectral imaging in close range applications. In: In: Halounova, L., Safar, V., Remondino, F., Hodac, J., Pavelka, K., Shortis, M., Rinaudo, F., Scaino, M., Boehm, J., RiekeZapp, D. (Eds.), XXIII ISPRS Congress, Commission V 41. pp. 865–870.
- Kurz, T.H., Buckley, S.J., Howell, J.A., 2013. Close-range hyperspectral imaging for geological field studies: workflow and methods. *Int. J. Remote Sens.* 34 (5), 1798–1822.
- Lee, C.M., Cable, M.L., Hook, S.J., Green, R.O., Ustin, S.L., Mandl, D.J., Middleton, E.M., 2015. An introduction to the NASA Hyperspectral InfraRed Imager (HyspIRI) mission and preparatory activities. *Remote Sens. Environ.* 167, 6–19.
- Linker, R., 2004. Waveband selection for determination of nitrate in soil using mid-infrared attenuated total reflectance spectroscopy. *Appl. Spectrosc.* 58 (11), 1277–1281.
- Majeke, B., van Aardt, J.A.N., Cho, M.A., 2008. Imaging spectroscopy of foliar biochemistry in forestry environments. *South. For.* 70 (3), 275–285.
- Matteson, A., Herron, M.M., 1993. End-member feldspar concentrations determined by FTIR spectral-analysis. *J. Sediment. Petrol.* 63 (6), 1144–1148.
- McClellan, W.D., Holm, R.E., Orr, D.G., Meiners, J.P., 1963. Spectral reflectance studies on plants. *Phytopathology* 53 (7) 747- & .
- McLellan, T.M., Aber, J.D., Martin, M.E., Melillo, J.M., Nadelhoffer, K.J., 1991. Determination of nitrogen, lignin, and cellulose content of decomposing leaf material by near-infrared reflectance spectroscopy. *Can. J. For. Res.–Revue Canadienne De Recherche Forestiere* 21 (11), 1684–1688.
- Milton, E.J., Schaepman, M.E., Anderson, K., Kneubuhler, M., Fox, N., 2009. Progress in field spectroscopy. *Remote Sens. Environ.* 113, S92–S109.
- Minasny, B., McBratney, A.B., Bellon-Maurel, V., Roger, J.M., Gobrecht, A., Ferrand, L., Joalland, S., 2011. Removing the effect of soil moisture from NIR diffuse reflectance spectra for the prediction of soil organic carbon. *Geoderma* 167–168, 118–124.
- Montero, I.C., Brimhall, G.H., Alpers, C.N., Swayze, G.A., 2005. Characterization of waste rock associated with acid drainage at the Penn Mine, California, by ground-based visible to short-wave infrared reflectance spectroscopy assisted by digital mapping. *Chem. Geol.* 215 (1–4), 453–472.
- Moody, A., Woodcock, C.E., 1995. The influence of scale and the spatial characteristics of landscapes on land-cover mapping using remote sensing. *Landsc. Ecol.* 10 (6), 363–379.
- Mouazen, A.M., Karoui, R., Deckers, J., De Baerdemaeker, J., Ramon, H., 2007. Potential of visible and near-infrared spectroscopy to derive colour groups utilising the Munsell soil colour charts. *Biosyst. Eng.* 97 (2), 131–143.
- Mutanga, O., Skidmore, A.K., Kumar, L., Ferwerda, J., 2005. Estimating tropical pasture quality at canopy level using band depth analysis with continuum removal in the visible domain. *Int. J. Remote Sens.* 26 (6), 1093–1108.
- Nocita, M., Stevens, A., van Wesemael, B., Aitkenhead, M., Bachmann, M., Barthes, B., Ben Dor, E., Brown, D.J., Clairotte, M., Csorba, A., Dardenne, P., Dematte, J.A.M., Genot, V., Guerrero, C., Knadel, M., Montanarella, L., Noon, C., Ramirez-Lopez, L., Robertson, J., Sakai, H., Soriano-Disla, J.M., Shepherd, K.D., Stenberg, B., Towett, E.K., Vargas, R., Wetterlind, J., 2015. Soil spectroscopy: an alternative to wet chemistry for soil monitoring. In: In: Sparks, D.L. (Ed.), *Advances in Agronomy*, vol. 132. Elsevier Academic Press Inc, San Diego, pp. 139–159.
- Norris, K.H., Barnes, R.F., Moore, J.E., Shenk, J.S., 1976. Predicting forage quality by infrared reflectance spectroscopy. *J. Anim. Sci.* 43 (4), 889–897.
- Pereira, H.M., Ferrier, S., Walters, M., Geller, G.N., Jongman, R.H.G., Scholes, R.J., Bruford, M.W., Brummitt, N., Butchart, S.H.M., Cardoso, A.C., Coops, N.C., Dulloo, E., Faith, D.P., Freyhof, J., Gregory, R.D., Heip, C., Hoft, R., Hurtt, G., Jetz, W., Karp, D.S., McGeoch, M.A., Obura, D., Onoda, Y., Pettorelli, N., Reyers, B., Sayre, R., Scharlemann, J.P.W., Stuart, S.N., Turak, E., Walpole, M., Wegmann, M., 2013. Essential biodiversity variables. *Science* 339, 277–278.
- Pettorelli, N., Owen, H.J.F., Duncan, C., 2016. How do we want Satellite Remote Sensing to support biodiversity conservation globally? *Methods Ecol. Evol.* 7 (6), 656–665.
- Pronca, V., Martin, L.J., Pereira, H.M., Fernandez, M., McRae, L., Belnap, J., Bohm, M., Brummitt, N., Garcia-Moreno, J., Gregory, R.D., Honrado, J.P., Jurgens, N., Opige, M., Schmeller, D.S., Tiago, P., van Swaay, C.A.M., 2017. Global biodiversity monitoring: from data sources to essential biodiversity variables. *Biol. Conserv.* 213, 256–263.
- Quattrochi, D.A., Atkinson, P.M., 1999. Introduction to this special issue on Geostatistics and Scaling of Remote Sensing and Spatial Data. *Photogramm. Eng. Remote Sens.* 65 (1), 40.
- Quattrochi, D.A., Goodchild, M.F., 1997. *Scale in Remote Sensing and GIS*. CRC Press, Boca Raton, Florida, US, pp. 406.
- Raffy, M., 1992. Change of scale in models of remote sensing – a general method for spatialisation of models. *Remote Sens. Environ.* 40 (2), 101–112.
- Ramoelo, A., Skidmore, A.K., Cho, M.A., Mathieu, R., Heitkonig, I.M.A., Dudeni-Thone, N., Schlerf, M., Prins, H.H.T., 2013. Non-linear partial least square regression increases the estimation accuracy of grass nitrogen and phosphorus using in situ hyperspectral and environmental data. *ISPRS J. Photogramm. Remote Sens.* 82, 27–40.
- Rast, M., Bezy, J.L., Bruzzi, S., 1999. The ESA medium resolution imaging spectrometer MERIS – a review of the instrument and its mission. *Int. J. Remote Sens.* 20 (9), 1681–1702.
- Rathod, P.H., Rossiter, D.G., Noomen, M.F., van der Meer, F.D., 2013. Proximal spectral sensing to monitor phytoremediation of metal-contaminated soils. *Int. J. Phytoremediation* 15 (5), 405–426.
- Reich, G., 2005. Near-infrared spectroscopy and imaging: basic principles and pharmaceutical applications. *Adv. Drug Deliv. Rev.* 57 (8), 1109–1143.
- Ren, H.Y., Zhuang, D.F., Singh, A.N., Pan, J.J., Qiu, D.S., Shi, R.H., 2009. Estimation of As and Cu contamination in agricultural soils around a mining area by reflectance spectroscopy: a case study. *Pedosphere* 19 (6), 719–726.
- Roggo, Y., Chalus, P., Maurer, L., Lema-Martinez, C., Edmond, A., Jent, N., 2007. A review of near infrared spectroscopy and chemometrics in pharmaceutical technologies. *J. Pharm. Biomed. Anal.* 44 (3), 683–700.
- Rossel, R.A.V., Behrens, T., Ben-Dor, E., Brown, D.J., Dematte, J.A.M., Shepherd, K.D., Shi, Z., Stenberg, B., Stevens, A., Adamchuk, V., Aichi, H., Barthes, B.G., Bartholomeus, H.M., Bayer, A.D., Bernoux, M., Bottcher, K., Brodsky, L., Du, C.W., Chappell, A., Fouad, Y., Genot, V., Gomez, C., Grunwald, S., Gubler, A., Guerrero, C., Hedley, C.B., Knadel, M., Morras, H.J.M., Nocita, M., Ramirez-Lopez, L., Roudier, P., Campos, E.M.R., Sanborn, P., Selltito, V.M., Sudduth, K.A., Rawlins, B.G., Walter, C., Winowiecki, L.A., Hong, S.Y., Ji, W., 2016. A global spectral library to characterize the world's soil. *Earth Sci. Rev.* 155, 198–230.
- Rossel, R.A.V., Walvoort, D.J.J., McBratney, A.B., Janik, L.J., Skjemstad, J.O., 2006. Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties. *Geoderma* 131 (1–2), 59–75.
- Salisbury, J.W., Walter, L.S., Vergo, N., D'Aria, D.M., 1991. *Infrared (2.1–25 Micrometers) Spectra of Minerals*. Johns Hopkins University Press, pp. 294.
- Schodlok, M.C., Whitbourn, L., Huntington, J., Mason, P., Green, A., Berman, M., Coward, D., Connor, P., Wright, W., Jolivet, M., Martinez, R., 2016. HyLogger-3, a visible to shortwave and thermal infrared reflectance spectrometer system for drill core logging: functional description. *Aust. J. Earth Sci.* 63 (8), 929–940.
- Serrano, L., Penueles, J., Ustin, S.L., 2002. Remote sensing of nitrogen and lignin in Mediterranean vegetation from AVIRIS data: decomposing biochemical from structural signals. *Remote Sens. Environ.* 81 (2–3), 355–364.
- Shepherd, K.D., Walsh, M.G., 2002. Development of reflectance spectral libraries for characterization of soil properties. *Soil Sci. Soc. Am. J.* 66 (3), 988–998.
- Shrestha, D.P., Margate, D.E., van der Meer, F., Anh, H.V., 2005. Analysis and classification of hyperspectral data for mapping land degradation: an application in southern Spain. *Int. J. Appl. Earth Obs. Geoinf.* 7 (2), 85–96.
- Siebielec, G., McCarthy, G.W., Stuczynski, T.I., Reeves, J.B., 2004. Near- and mid-infrared diffuse reflectance spectroscopy for measuring soil metal content. *J. Environ. Qual.* 33 (6), 2056–2069.
- Sobrinho, J.A., Mattar, C., Pardo, P., Jimenez-Munoz, J.C., Hook, S.J., Baldrige, A., Ibanez, R., 2009. Soil emissivity and reflectance spectra measurements. *Appl. Opt.* 48 (19), 3664–3670.
- Stevens, A., van Wesemael, B., Bartholomeus, H., Rosillon, D., Tychon, B., Ben-Dor, E., 2008. Laboratory, field and airborne spectroscopy for monitoring organic carbon content in agricultural soils. *Geoderma* 144 (1–2), 395–404.
- Stoll, M.P., Laurila, T., Buschmann, C., Moreno, J., Court, A., Moya, I., Ieee, 2003. The FLEX-Fluorescence Explorer mission project: motivations and present status of preparatory activities, New York, Ieee, Igarss 2003. IEEE International Geoscience and Remote Sensing Symposium, Vols I – Vii, Proceedings: Learning from Earth's Shapes and Sizes 585–587.
- Stoner, E.R., Baumgardner, M.F., Weismiller, R.A., Biehl, L.L., Robinson, B.F., 1980. Extension of laboratory-measured soil spectra to field conditions. *Soil Sci. Soc. Am. J.*

- 44 (3), 572–574.
- Stuffer, T., Kaufmann, C., Hofer, S., Forster, K.P., Schreier, G., Mueller, A., Eckardt, A., Bach, H., Penne, B., Benz, U., Haydn, R., 2007. The EnMAP hyperspectral imager—an advanced optical payload for future applications in Earth observation programmes. *Acta Astronaut.* 61 (1–6), 115–120.
- Tappert, M., Rivard, B., Giles, D., Tappert, R., Mauger, A., 2011. Automated drill core logging using visible and near-infrared reflectance spectroscopy: a case study from the Olympic Dam IOCG deposit, South Australia. *Econ. Geol.* 106 (2), 289–296.
- Tathavadar, V.D., Antony, M.P., Jha, A., 2004. An investigation of the mineralogical properties of chemical grade chromite minerals. *Scand. J. Metall.* 33 (2), 65–75.
- Ulusoy, Y., Tekin, Y., Tumsavas, Z., Mouazen, A.M., 2016. Prediction of soil cation exchange capacity using visible and near infrared spectroscopy. *Biosyst. Eng.* 152, 79–93.
- Vagen, T.G., Shepherd, K.D., Walsh, M.G., 2006. Sensing landscape level change in soil fertility following deforestation and conversion in the highlands of Madagascar using Vis-NIR spectroscopy. *Geoderma* 133 (3–4), 281–294.
- Van der Meer, F., 1995. Spectral reflectance of carbonate mineral mixtures and bidirectional reflectance theory: quantitative analysis techniques for application in remote sensing. *Remote Sens. Rev.* 13, 67–94.
- Van der Meer, F., 2012. Remote-sensing image analysis and geostatistics. *Int. J. Remote Sens.* 33 (18), 5644–5676.
- Van der Meer, F., Kopackova, V., Koucká, L., van der Werff, H.M.A., van Ruitenbeek, F.J.A., Bakker, W.H., 2018. Wavelength feature mapping as a proxy to mineral chemistry for investigating geologic systems: an example from the Rodalquilar epithermal system. *Int. J. Appl. Earth Obs. Geoinf.* 64, 237–248.
- van Ruitenbeek, F.J.A., Bakker, W.H., van der Werff, H.M.A., Zegers, T.E., Oosthoek, J.H.P., Omer, Z.A., Marsh, S.H., van der Meer, F.D., 2014. Mapping the wavelength position of deepest absorption features to explore mineral diversity in hyperspectral images. *Planet. Space Sci.* 101, 108–117.
- Van Ruitenbeek, F.J.A., Cudahy, T., Hale, M., van der Meer, F.D., 2005. Tracing fluid pathways in fossil hydrothermal systems with near-infrared spectroscopy. *Geology* 33 (7), 597–600.
- Van Ruitenbeek, F.J.A., Debba, P., van der Meer, F.D., Cudahy, T., van der Meijde, M., Hale, M., 2006. Mapping white micas and their absorption wavelengths using hyperspectral band ratios. *Remote Sens. Environ.* 102 (3–4), 211–222.
- Vasques, G.M., Grunwald, S., Sickman, J.O., 2009. Modeling of soil organic carbon fractions using visible-near-infrared spectroscopy. *Soil Sci. Soc. Am. J.* 73 (1), 176–184.
- Verhoef, W., 1984. Light-scattering by leaf layers with application to canopy reflectance modeling – the SAIL model. *Remote Sens. Environ.* 16 (2), 125–141.
- Waruru, B.K., Shepherd, K.D., Ndegwa, G.M., Kamoni, P.T., Sila, A.M., 2014. Rapid estimation of soil engineering properties using diffuse reflectance near infrared spectroscopy. *Biosyst. Eng.* 121, 177–185.
- Wessman, C.A., Aber, J.D., Peterson, D.L., Melillo, J.M., 1988a. Foliar analysis using near-infrared reflectance spectroscopy. *Can. J. For. Res.* 18 (1), 6–11.
- Wessman, C.A., Aber, J.D., Peterson, D.L., Melillo, J.M., 1988b. Remote-sensing of canopy chemistry and nitrogen cycling in temperate forest ecosystems. *Nature* 335 (6186), 154–156.
- Wold, S., Ruhe, A., Wold, H., Dunn, W.J., 1984. The collinearity problem in linear regression – the partial least squares (PLS) approach to generalized inverses. *Siam J. Sci. Stat. Comput.* 5 (3), 735–743.
- Wold, S., Sjostrom, M., Eriksson, L., 2001. PLS-regression: a basic tool of chemometrics. *Chemom. Intell. Lab. Syst.* 58 (2), 109–130.
- Woodcock, C., Strahler, A.H., 1987. The factor scale in remote sensing. *Remote Sens. Environ.* 21, 311–332.
- Wu, H., Li, Z.L., 2009. Scale issues in remote sensing: a review on analysis. *Process. Model.: Sens.* 9 (3), 1768–1793.
- Wu, J., Bai, Q.L., Su, S.B., Chen, S.J., Meng, Q.X., Yan, Y.L., 2005a. Near-infrared reflectance spectroscopy analysis of cellulose content in corn stalk: chinese. *J. Anal. Chem.* 33 (10), 1421–1423.
- Wu, Y.Z., Chen, J., Ji, J.F., Tian, Q.J., Wu, X.M., 2005b. Feasibility of reflectance spectroscopy for the assessment of soil mercury contamination. *Environ. Sci. Technol.* 39 (3), 873–878.
- Yitagesu, F.A., van der Meer, F., van der Werff, H., Hecker, C., 2011. Spectral characteristics of clay minerals in the 2.5–14 μm wavelength region. *Appl. Clay Sci.* 53 (4), 581–591.
- Yitagesu, F.A., van der Meer, F., van der Werff, H., Zigterman, W., 2009. Quantifying engineering parameters of expansive soils from their reflectance spectra. *Eng. Geol.* 4, 151–160.
- Ymeti, I., van der Werff, H., Shrestha, D.P., Jetten, V.G., Lievens, C., van der Meer, F., 2017. Using color, texture and object-based image analysis of multi-temporal camera data to monitor soil aggregate breakdown. *Sensors* 17, 6.
- Yoder, B.J., Pettigrewcrosby, R.E., 1995. Predicting nitrogen and chlorophyll content from reflectance spectra (400–2500 nm) at leaf and canopy scales. *Remote Sens. Environ.* 53 (3), 199–211.
- Zaini, N., van der Meer, F., van der Werff, H., 2014. Determination of carbonate rock chemistry using laboratory-based hyperspectral imagery. *Remote Sens.* 6 (5), 4149–4172.
- Zaini, N., van der Meer, F., van Ruitenbeek, F., de Smeth, B., Amri, F., Lievens, C., 2016. An alternative quality control technique for mineral chemistry analysis of Portland cement-grade limestone using shortwave infrared spectroscopy. *Remote Sens.* 8, 11.