



Estimating soil zinc concentrations using reflectance spectroscopy



Weichao Sun^{a,b}, Xia Zhang^{a,*}

^a Institute of Remote Sensing and Digital Earth, Chinese Academy of Sciences, No.20 Datun Road, Chaoyang District, Beijing 100101, China

^b University of Chinese Academy of Sciences, Yuquan Street, Shijingshan District, Beijing 100049, China

ARTICLE INFO

Article history:

Received 18 November 2016

Received in revised form 23 January 2017

Accepted 24 January 2017

Keywords:

Reflectance spectroscopy

Soil heavy metal

Organic matter

Clay minerals

Band selection

ABSTRACT

Soil contamination by heavy metals has been an increasingly severe threat to nature environment and human health. Efficiently investigation of contamination status is essential to soil protection and remediation. Visible and near-infrared reflectance spectroscopy (VNIRS) has been regarded as an alternative for monitoring soil contamination by heavy metals. Generally, the entire VNIR spectral bands are employed to estimate heavy metal concentration, which lacks interpretability and requires much calculation. In this study, 74 soil samples were collected from Hunan Province, China and their reflectance spectra were used to estimate zinc (Zn) concentration in soil. Organic matter and clay minerals have strong adsorption for Zn in soil. Spectral bands associated with organic matter and clay minerals were used for estimation with genetic algorithm based partial least square regression (GA-PLSR). The entire VNIR spectral bands, the bands associated with organic matter and the bands associated with clay minerals were incorporated as comparisons. Root mean square error of prediction, residual prediction deviation, and coefficient of determination (R^2) for the model developed using combined bands of organic matter and clay minerals were $329.65 \text{ mg kg}^{-1}$, 1.96 and 0.73, which is better than $341.88 \text{ mg kg}^{-1}$, 1.89 and 0.71 for the entire VNIR spectral bands, $492.65 \text{ mg kg}^{-1}$, 1.31 and 0.40 for the organic matter, and $430.26 \text{ mg kg}^{-1}$, 1.50 and 0.54 for the clay minerals. Additionally, in consideration of atmospheric water vapor absorption in field spectra measurement, combined bands of organic matter and absorption around 2200 nm were used for estimation and achieved high prediction accuracy with R^2 reached 0.640. The results indicate huge potential of soil reflectance spectroscopy in estimating Zn concentrations in soil.

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1. Introduction

Soil is a complex heterogeneous combination of mineral, organic and fluid matter that comprises mineral soils (Stoner and Baumgardner, 1981). Heavy metals in soil derive from either a parent material or anthropogenic deposition. Soil acts as a buffer between the source of pollution and the living organism due to its remarkable ability to immobilize metal ions through various kinds of adsorption mechanism (Bradl, 2004). The adsorbed metals may be released if the corresponding equilibria are altered by natural or anthropogenic changes in environment conditions. Contaminant elements, such as copper (Wang et al.), nickel (Ni) and zinc (Zn), are essential micronutrients at very low concentrations, but are toxic at high levels. Other elements, like cadmium (Cd) and mercury (Yeganeh et al., 2013), are toxic even if their concentrations are very low. Moreover, heavy metals tend to accumulate in the living

organism, which may increase the adverse effects. Therefore, it's significant to monitor heavy metal concentrations in soil.

The conventional method of investigating soil heavy metal contamination is based on regular field samplings and subsequent chemical analyses in the laboratory, followed by geo-statistical interpolation to exhibit the spatial distribution of heavy metals (Leenaers et al., 1990). However, this method may be costly and time-consuming as a result of the intensive soil samplings in the field and the analyses in the laboratory (Shi et al., 2014). Soil reflectance is a cumulative property which derives from inherent spectral behavior of the heterogeneous combination of soil physical and chemical properties. Studies have revealed the relative contribution of soil constituents such as organic matter, iron oxide and clay minerals to soil reflectance spectra (Fidencio et al., 2002; Kooistra et al., 2001; Wu et al., 2007; Xu et al., 1995). Visible and near-infrared spectroscopy (VNIRS) has been applied in soil sciences for more than 20 years. The VNIRS technology has several distinct advantages over conventional soil investigation method, including non-destructive, highly reproducible, rapid, cheap when extensive measurements are need, small quantity of samples is needed for analysis (Guerrero et al., 2010). Transition elements such

* Corresponding author.

E-mail addresses: sunwc@radi.ac.cn (W. Sun), zhangxia@radi.ac.cn (X. Zhang).

as Ni, Cu, Co, and Cr with an unfilled 'd' shell, can exhibit absorption features due to crystal field effects in visible and near-infrared (VNIR) region (Burns, 1993; Clark, 1999). Zn is not spectrally active in VNIR region. However, regardless of the absorption features, heavy metal elements cannot be detected with reflectance spectroscopy at low concentrations (Wu et al., 2007). Although heavy metals at low concentration levels do not have spectral features within VNIR region, prediction for the featureless element concentrations in soil can be made via correlation with organic matter, clay minerals and iron oxide (BenDor et al., 1997; Rathod et al., 2013; Wu et al., 2007).

The entire VNIR spectral bands were used to estimate Zn concentrations in river floodplains and the result indicate that Zn concentration in a sediment largely depends on the content of clay and organic matter (Kooistra et al., 2001). The entire VNIR spectral bands were also employed in the estimation of Zn concentrations in agricultural soils and the result suggests that the correlation between Zn and total iron (including active and residual iron) is the major mechanism for investigating Zn concentration (Wu et al., 2007; Wu et al., 2005). In order to select meaningful bands for Zn concentration estimation, continuum removal and genetic algorithm (GA) were applied to the entire VNIR spectral bands (Choe et al., 2008; Wang et al., 2014).

The risk of Zn contamination depends on the concentration of pollutant in the soil solution, which in turn depends on the adsorption-desorption equilibria that govern the partition of pollutant between soil solution and soil solids, especially between soil solution and soil colloids (Arias et al., 2005). The most important colloids related to heavy metal adsorption in soils are organic matter, clay minerals and iron oxide (Gerritse and Vandriel, 1984; Shuman, 1988; Spark et al., 1995). In the case of whole soils, studies on the adsorption and desorption of heavy metals should consider the potential competition between heavy metals for binding sites (Covelo et al., 2007a). Study on simultaneous adsorption and desorption of Cd, Cr, Cu, Ni, Pb and Zn indicates that Zn was strongly adsorbed by soils with high organic matter contents and appreciable vermiculite contents (Covelo et al., 2007b), which is consistent with the conclusion that adsorption of Zn is influenced by factors such as pH, clay mineral content, soil organic matter (Bradl, 2004). Another sorption experiment designed to explore association of individual soil constituents and heavy metals (Cu, Zn, and Pb) revealed that, under competitive situation, Zn was sorbed mostly on soil mineral constituents, mainly vermiculite and montmorillonite (Sipos et al., 2009).

Application of entire VNIR spectral range (VNIR-SR, defined as 400–2400 nm in this study) in estimating Zn concentration in soil lacks interpretability and requires huge calculation cost. The efforts to select the meaningful bands associated with Zn in soil are insufficient for the application. More efforts are needed to improve the interpretability and reduce calculation cost in estimating Zn concentrations using reflectance spectroscopy. Thus, in this study, soil reflectance spectroscopy associated with organic matter and clay minerals was used to estimate Zn concentrations in soil with GA based partial least square regression (PLSR-GA).

2. Material and methods

2.1. Soil sampling and chemical analysis

The study area was in Qingjiang Village, Chenzhou City, Hunan Province, China. The Qingjiang lead/zinc mine which is one of the six biggest mines in the basin of the Dong River is located in the village. Mining activity is a chief source of metals entering the environment, since mine tailing and wastewater are created and dust is emitted in the process of mining exploitation and ore concen-

trating. On August 25th, 1985, the mine tailing dam of Chezhou lead/zinc mine collapsed because of heavy rain, which resulted in a strip of farmland about 400 m in wide on both side of the Dong River channel was covered with a thick layer of black sludge. Metal concentration analysis indicated that Zn is predominantly elevated in all the soil sampled collected along the Dong River in 2002, and the highest Zn concentration was 1252 mg kg⁻¹ (Liu et al., 2005).

Soil sampling was conducted in Qingjiang Village. Eighty-three topsoil samples (depth 0–20 cm) were collected in the area of 113°17'17.76"E to 113°17'36.07"E and 25°45'39.29"N to 25°46'1.13"N, at the altitude of 335 m to 451 m. The study area and sampling sites are shown in Fig. 1.

The collected soil samples were air-dried at 20 °C and sieved through a 2 mm polyethylene sieve to remove stones and other large debris. The samples were then ground into fine particles. Zn concentrations in the collected soil samples were determined using acid digestion method and measured by flame atomic absorption spectrometry, as recommended by the Environment Quality Standard for Soil which was released by Ministry of Environment Protection of China in 1996.

2.2. Spectral measurement and preprocessing

Soil spectra were measured by a portable spectrometer PSR-3500 (Spectral Evolution Inc., Lawrence, MA, USA) which covers a spectral range of 350–2500 nm and offers spectral resolutions of 3.5 nm at 700 nm, 10 nm at 1500 nm and 7 nm at 2100 nm. Spectral intervals were 1.5 nm at 700 nm, 3.8 nm at 1500 nm and 2.5 nm at 2100 nm. A 50 W halogen lamp at an angle of 30° from nadir was mounted at 60 cm above the center of the samples as stable light source in a dark room. The spectrometer was fixed above the center of the soil samples. Each sample was uniformly tiled on a black cloth and was measured five times. The average spectrum was calculated and used in further processing. The spectrometer was calibrated after every three samples using a white BaSO₄ panel.

Generally, wavelengths on the fringe of the VNIR region for the spectrometer have a relatively low signal-to-noise ratio. To reduce noise and calculation cost, spectral bands at intervals of 350–399 nm and 2400–2500 nm were removed with reference to previous studies (Chen et al., 2015; Kooistra et al., 2001). Nine spectra were found to have reflectance more than or close to 100% in several bands due to measurement error after checking the 83 soil spectra. The 9 reflectance spectra were therefore removed to reduce the estimation error.

The remaining 74 soil reflectance spectra in Fig. 2 show that wavelengths in the VNIR region of 400–2400 nm are affected by noise to different extents. The disturbance in the visible region was relatively slight, but the disturbance increased for bands beyond the visible region, especially at the interval of 1800–2400 nm. A piecewise Savitzky-Golay (SG) smoothing model was designed to reduce the noise brought in the process of spectral measurement and to preserve spectral information of soil samples simultaneously. In piecewise SG smoothing process, seven points and a quadratic polynomial were used in the visible region, and 14 points and a quadratic polynomial were adopted for the region beyond.

2.3. Extracting spectral bands correlated with Zn in soil

2.3.1. Spectral bands correlated with Zn

The adsorption of Zn on spectrally active soil constituents (organic matter, iron oxide, and clay minerals) provides a mechanism for estimating Zn concentrations in soil using reflectance spectroscopy. Studies have revealed that organic matter and clay minerals have strong adsorption for Zn in soil (Bradl, 2004; Covelo et al., 2007b). A chemical sequential extraction experiment on soil samples collected from southern China shows that: i) the presence

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