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Predicting nickel concentration in soil using reflectance spectroscopy associated with organic matter and clay minerals

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ABSTRACT

Heavy metal contamination in soil has become a serious environmental problem. Visible and near-infrared reflectance spectroscopy (VNIRS) is recognized as an alternative to rapidly predict heavy metal concentration in soil. The correlation between soil spectrally active constituents and heavy metals provides a mechanism for the prediction. Generally, the entire VNIR spectral region (VNIR-SR) without discrimination is used. Considering the adsorption and retention of heavy metals on soil spectrally active constituents, a method was proposed to predict heavy metal concentration in soil using VNIRS. Organic matter and clay minerals have strong sorption and retention for Ni in soil. Therefore, the spectral bands associated with organic matter and clay minerals were used to predict nickel (Ni) concentration to validate the proposed method. In this study, two sets of reflectance spectra of soil samples collected in Chenzhou and Hengyang, Hunan Province, China were used. The prediction model was calibrated with a combination of genetic algorithm and partial least squares regression (GA-PLSR). In Chenzhou, the ratio of prediction to deviation (RPD) and the coefficient of determination (R^2) were improved from 1.566 and 0.577 to 2.139 and 0.773 by the prediction using the spectral bands associated with organic matter and clay minerals compared with the prediction using the entire VNIR-SR. The RPD and R^2 were improved from 1.805 and 0.672 to 3.144 and 0.892 by the proposed method in Hengyang. To further validate the proposed method, the soil samples from Chenzhou were reallocated to calibration and validation sets according to Ni concentration. The RPD and R^2 were improved from 1.193 and 0.267 to 2.396 and 0.818 by using the spectral bands associated with organic matter and clay minerals. The results indicate that the proposed method is effective in predicting Ni concentration and has the potential to predict other heavy metals in soil.

1. Introduction

Soil contamination by heavy metals has been a severe environmental problem, particularly for countries undergoing rapid industrialization and urbanization (Wong et al., 2002). Nickel (Ni) is an essential micronutrient at very low concentrations. But it is toxic at high concentrations (Yeganeh et al., 2013). The risk associated with Ni in soil depends mainly on its potential ability to enter food chains. Chronic intake of Ni, even at low levels, may adversely affect human health due to its accumulation. Studies have shown an increased incidence of cancers to be associated with chronic exposure to Ni (Denkhaus and Salnikow, 2002; Kasprzak, 2003). Therefore, it is essential to investigate Ni concentration in soil.

The conventional method to obtain heavy metal concentration in soil is based on field sampling and subsequent laboratory chemical analysis (Leenaers et al., 1990; Steiger et al., 1996). However, the conventional method is time-consuming and expensive, particularly for extensive soil sampling and chemical analysis in large areas. Additionally, it is difficult to describe the dynamics of the contaminant elements over a large scale based on limited soil samples, due to the spatial and temporal limitations of the conventional method.

Visible and near-infrared spectroscopy (VNIRS) of soil is a cumulative property of the heterogeneous combination of organic matter, soil moisture, particle size and distribution, iron oxide, soil mineralogy, and parent material. Compared with conventional analytical methods, the spectroscopic method is non-destructive, rapid, and cost-effective (Shi et al., 2014). VNIRS can be measured using portable spectrometers in field and imaging spectrometers in both field and different platforms, which is the primary advantage of the spectroscopic method. VNIRS has been used to predict heavy metal concentration in soil since 1997 (Malley and Williams, 1997). The prediction of Ni concentration in soil using VNIRS was conducted in suburban agricultural soil (Wu et al.,

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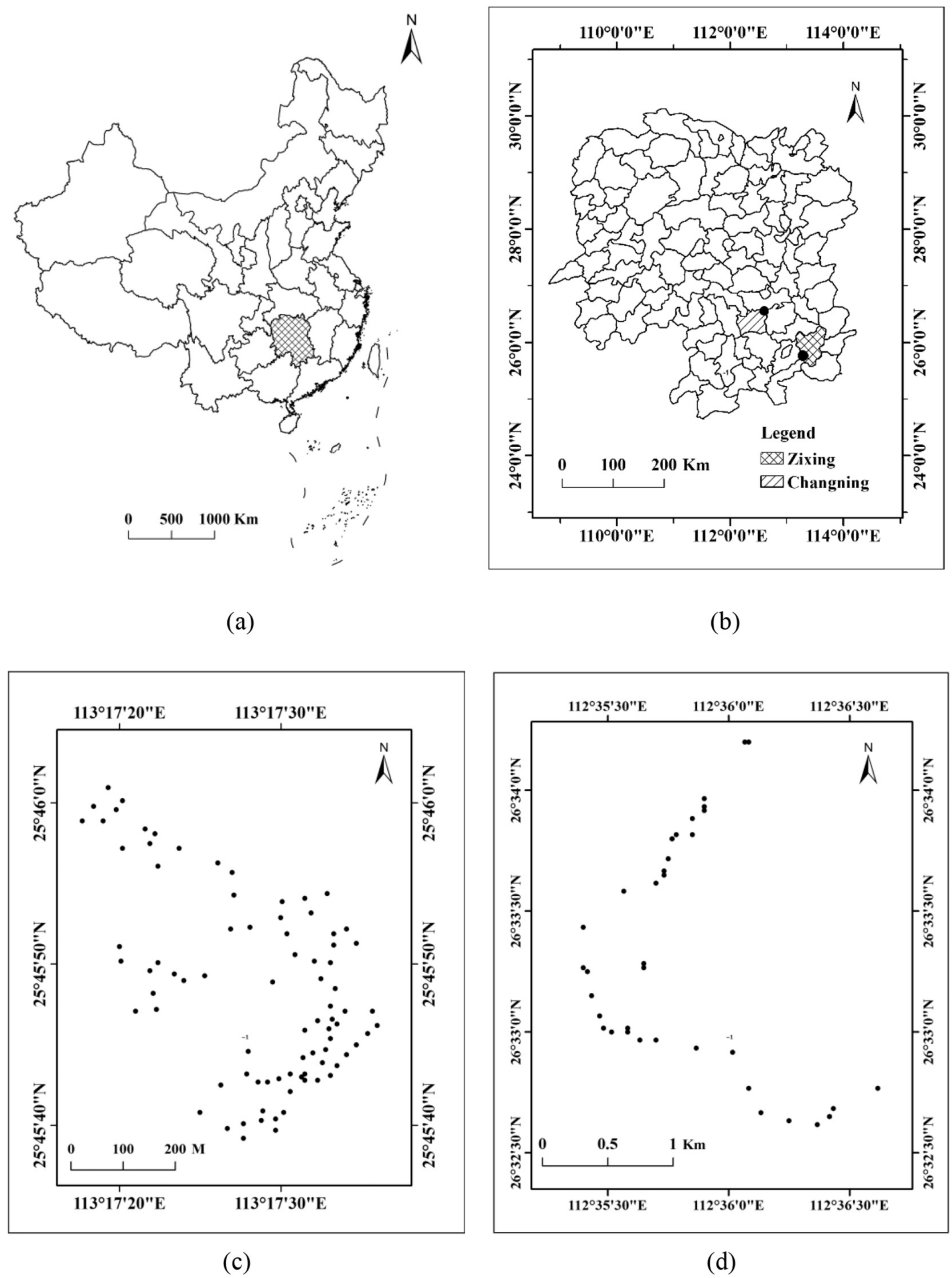

Fig. 1. Study areas and sampling sites. Hunan Province is labeled with crosshatch in Fig. 1(a). Zixing, Chenzhou City and Changning, Hengyang City are labeled with crosshatch in Fig. 1(b), the corresponding two sampling sites are marked with solid black circle in the two study areas. The detailed sampling sites in Chenzhou and Hengyang are shows in Fig. 1(c) and (d).

2007; Wu et al., 2005) and river sediment (Song et al., 2013).

Although heavy metals in soil cannot be identified directly with reflectance spectroscopy at low concentrations (Wu et al., 2005), increased input of heavy metals is absorbed by iron oxides, organic matter, and clay minerals (Bradl, 2004; Vega et al., 2004). Studies have shown that iron oxides, organic matter, and clay minerals are spectrally active in VNIR (Ben-Dor and Banin, 1995; Kooistra et al., 2003; Liu and Chen, 2012; Madeira et al., 1997). Therefore, soil reflectance spectroscopy can be used to determine heavy metal concentration in soil based on the correlation between the contaminant elements and soil spectrally active constituents (Kemper and Sommer, 2002; Kooistra et al., 2001; Rathod et al., 2013). VNIRS is reported to be an alternative for monitoring soil contamination by heavy metals (Shi et al., 2014).

Generally, the entire VNIR spectral region (VNIR-SR) without discrimination is used in predicting heavy metal concentration (Chen et al., 2015; Song et al., 2013; Wang et al., 2014). The absorption and retention of heavy metals on soil spectrally active constituents varies with specific contaminant element and soil condition. Considering spectral characteristics of soil spectrally active soil constituents, it can be concluded that the contribution of spectral bands to prediction of