



Estimation of weathering indices using spectral reflectance over visible to mid-infrared region



Biswajita Mohanty, Abhinav Gupta, Bhabani S. Das *

Agricultural and Food Engineering Department, Indian Institute of Technology Kharagpur, WB 721302, India

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ABSTRACT

A new approach to estimate weathering indices (WIs) in soil was developed using proximally-sensed spectral reflectance over visible to shortwave-infrared (vis–NIR) and mid-infrared (MIR) region of electromagnetic spectrum. Partial-least-squares regression (PLSR) analysis was used to develop spectral algorithms for estimating twelve different WIs commonly used in geochemical literature. For each index, two different models were calibrated: 1) based on all the features in spectra and 2) based on the features obtained by variable importance projection, which we denote by vis–NIR_{vip}, MIR_{vip}, and (vis–NIR + MIR)_{vip}. The residual prediction deviation (RPD) was used for checking the robustness of spectral models. Results showed that the MIR reflectance data provided superior estimation capability for all WIs compared with the vis–NIR reflectance data with the best possible prediction obtained for index of laterization (IOL; RPD = 5.86) in the MIR and Mg Index (MgI; RPD = 2.43) in the vis–NIR approach. The highest RPD values of 3.12, 4.13, 3.78, 6.13, and 5.08 were obtained for chemical index of alteration (CIA), MgI, mafic index of alteration (MIA(O)), IOL, and weathering index of Parker (WIP), respectively, when the PLSR model was based on (vis–NIR + MIR)_{vip}. Best predictions were obtained when vis–NIR and MIR were combined and important spectral features were selected through variable importance projection (VIP) approach. Both vis–NIR and MIR technologies are available in the form of portable devices and are amenable for remote sensing mode of operation. This study demonstrates for the first time that the WI values in soil may be estimated in a rapid and non-destructive way in situ.

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1. Introduction

Chemical weathering changes the composition of top soil and produces large volumes of soluble materials that have the potential to change soil quality and pollute our water bodies (White et al., 2008). Weathering indices (WIs) are generally used for determining the severity of weathering. These indices are expressed as molar ratios of immobile to mobile mineral oxides present in soil. For example, the chemical index of alteration (CIA) is defined as the molar ratio of aluminum oxide (Al₂O₃) to the sum of the moles of Al₂O₃, sodium oxide (Na₂O), calcium oxide in the silicate mineral phase (CaO*) and potassium oxide (K₂O). Of about a dozen of these WIs (Table 1), CIA, weathering index of Parker (WIP) and mafic index of alteration (MIA) are frequently used (Nesbitt and Young, 1982; Li and Yang, 2010; JingQing and Yang, 2012; Fiantis et al., 2010; Bowen et al., 2013; Babechuk et al., 2014). These oxide

phases in soils are generally estimated from the major elements (Si, Al, Fe, Mn, Mg, Ca, Na, P, K, and Ti) measured through X-ray fluorescence (XRF) spectrometry. Molar abundances of elemental fractions in the form of oxides (hereinafter, referred to as elemental oxides) are used for estimating WIs. The method is accurate but is time-consuming and expensive.

Over the last two decades, diffuse reflectance spectroscopy (DRS) in the vis–NIR (350–2500 nm) region has emerged as a rapid, non-invasive and high throughput technique for the estimation of several soil properties (Ben-Dor and Banin, 1995; Chang et al., 2001; Islam et al., 2003; Sarathjith et al., 2014a, b; Viscarra Rossel et al., 2006; Waiser et al., 2007). Several researchers have used vis–NIR spectra (Hunt, 1970; Hunt et al., 1973; Madejová et al., 2009) for the assessment of clay minerals in soils. Recently, Mulder et al. (2013) have shown that the wavelength region over 2100–2400 nm of vis–NIR spectra may be used for the quantification of mineral abundance of complex soil mixtures. Viscarra Rossel et al. (2006) also predicted the composition of mineral–organic mixes using UV–vis–NIR spectra. Ben-Dor and Banin (1994) predicted CaCO₃, Fe₂O₃, Al₂O₃, SiO₂, and loss on ignition (LOI) using 400–1100 nm region of reflectance spectrum. The MIR region of the spectra (wave number: 4000 to 400 cm^{−1}) has also been used for the quantitative assessment of clay minerals (Djomgoue and Njopwouo, 2013; Peltre et al., 2014; Saikia and Parthasarathy, 2010).

Abbreviations: WI, weathering index; Vis–NIR, visible and near-infrared region; MIR, mid-infrared; PLSR, partial-least-squares regression; RPD, residual prediction deviation; VIP, variable importance projection; XRF, X-ray fluorescence; DRS, diffuse reflectance spectroscopy; FTIR, Fourier transform infrared.

* Corresponding author.

E-mail address: bsdas@agfe.iitkgp.ernet.in (B.S. Das).

Table 1
Different weathering indices used in the literature.

Weathering indices	Formula	Reference
Chemical index of alteration (CIA)	$100 \left(\frac{\text{Al}_2\text{O}_3}{\text{Al}_2\text{O}_3 + \text{CaO} + \text{Na}_2\text{O} + \text{K}_2\text{O}} \right)$	Nesbitt and Young (1982)
Plagioclase index of alteration (PIA)	$100 \left(\frac{\text{Al}_2\text{O}_3 - \text{K}_2\text{O}}{\text{Al}_2\text{O}_3 + \text{CaO} + \text{Na}_2\text{O} - \text{K}_2\text{O}} \right)$	Fedo et al. (1995)
MgI	$100 \left(\frac{\text{Al}_2\text{O}_3}{\text{Al}_2\text{O}_3 + \text{MgO}} \right)$	Maynard (1992)
CALMAG	$100 \left(\frac{\text{Al}_2\text{O}_3}{\text{Al}_2\text{O}_3 + \text{CaO} + \text{MgO}} \right)$	Nordt and Driese (2010)
Mafic index of alteration (MIA(O))	$100 \left(\frac{\text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3}{\text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{MgO} + \text{CaO} + \text{Na}_2\text{O} + \text{K}_2\text{O}} \right)$	Babechuk et al. (2014)
Index of laterization (IOL)	$100 \left(\frac{\text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3}{\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3} \right)$	Schellmann (1981)
CIA-potassium removed (CIA-K)	$100 \left(\frac{\text{Al}_2\text{O}_3}{\text{Al}_2\text{O}_3 + \text{CaO} + \text{Na}_2\text{O}} \right)$	Sheldon et al. (2002)
MIA(O)-K	$100 \left(\frac{\text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3}{\text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{MgO} + \text{CaO} + \text{Na}_2\text{O}} \right)$	Babechuk et al. (2014)
Weathering index of Parker (WIP)	$100 \left(2 \left(\frac{\text{Na}_2\text{O}}{0.35} \right) + \left(\frac{\text{MgO}}{0.90} \right) + 2 \left(\frac{\text{K}_2\text{O}}{0.25} \right) + 2 \left(\frac{\text{CaO}^*}{0.70} \right) \right)$	Parker (1970)
Silica to sesquioxide ratio (SSr)	$\left(\frac{\text{SiO}_2}{\text{TiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3} \right)$	Singh et al. (1998)

Note: All the indices are calculated using oxide values in molar units except for IOL, where oxide values are used in anhydrous weight % units.

Although elemental oxides have been frequently estimated by the diffuse reflectance spectroscopy (DRS) approach, limited studies have been reported on the use of DRS for studying weathering indices. Recently, Baptista et al. (2011) estimated the weathering index Ki (molar ratio of SiO₂ to Al₂O₃) using the band reflectance values at wavelengths of 2127, 2176, 2196, 2226, 2266, and 2296 nm derived from the AVIRIS data and showed a linear relationship between Ki and mineral fractions of kaolinite and gibbsite. More recently, Demattê and Terra (2014) estimated the weathering indices Ki and Kr to characterize weathering intensities along a topo-sequence. To the best of our knowledge, spectral algorithms for different WIs based on vis–NIR or MIR spectra have not been reported in the literature.

The DRS approach is primarily used for estimating different soil constituents that have a direct bearing on the electromagnetic energy a soil intercepts. Recently, Sarathjith et al. (2014a) have used the DRS approach for estimating aggregate size distribution parameters, which characterize a structural property of soil. Weathering indices are also a measure of bulk property similar to aggregate size distribution and are influenced by soil forming factors such as climate, organism, relief, parent material and time. Sarathjith et al. (2014b) have shown that soil properties with no direct correspondence with electromagnetic energies may also be quantified in the DRS approach provided that such properties are correlated with primary chromophores in soils. The main objective of this study was to examine the suitability of vis–NIR and MIR reflectance spectroscopy for estimating different WIs as a rapid and non-destructive approach; WI represents a bulk property of soil similar to the aggregate size distribution. A database of soil spectra over visible to MIR region and XRF-measured elemental composition were used to build PLSR models for commonly reported WIs.

2. Materials and methods

2.1. Soil collection and analysis

A total of 415 soil samples from 148 locations (three different depths of 0–10 cm, 20–25 cm and 50–55 cm) were collected from West Bengal and the northern part of Odisha state (17°31'–22°27'N, 85°53'–87°30'E) located in the eastern fringe of the Peninsular eastern India (Fig. 1). A major part of the state of West Bengal lies within the lower Gangetic Plains which is one of the most extensive fluvio-deltaic sedimentary systems on earth (Mukherjee et al., 2009). Based on the relative degree of development, Singh et al. (1998) classified West Bengal soils into five Quaternary soil groups: Ganga Floodplain (age: 0.5 ka), Bhagirathi Plain and Old Ganga Plain (age: 1–1.5 ka), Barind Tract (Lower Level) and Damodar Deltaic Plain (age: 3–4 ka), Bhagirathi–Ajay

Plain and Ajay–Silai Plain (age: 5–6 ka), and Upland with Red Soils (age: 350–1000 ka). Upland red soils are the most weathered soils and are also called laterite soils (Niyogi, 1975). The National Bureau of Soil Survey and Land Use Planning (NBSS&LUP) at Nagpur has identified 81 Soil Series in West Bengal of which 60 are derived from alluvium, 15 from granite gneiss and remaining from schists, laterites and sandstone Nayak, 2001. Dominant minerals in the soils found within the state are illite, kaolinite, smectite and interstratified minerals (Ghosh et al., 1974; Singh et al., 1998). The northern part of Odisha has deposits of iron, manganese, chromite, gneisses, granite, limestone, gold, lead and zinc of Archean and Proterozoic age. The NBSS&LUP has recognized 112 Soil Series in Odisha out of which 75 are derived from granite gneiss, 27 from alluvium, 4 from quartzite and the remaining from laterite and khondalite type of parent material (Sarkar and Sah, 2005). Most of the soil samples collected from Odisha were adjacent to major river systems of Subarnarekha, Brahmani, Baitarani and Mahanadi and hence had alluvial origin. Alfisols and Inceptisols form the major Orders in both the States. A few soils of these two states have also been classified as Vertisols with vertic intergrades (Bhattacharyya et al., 2013). Soil samples were collected from areas with different land uses such as cultivated paddy fields, barren land and forests. Each sample was air-dried, ground and sifted through a 2 mm sieve and stored for the measurement of physical and chemical properties, mineralogy, and spectral reflectance.

Out of the 415 soil samples, elemental composition was determined for only 126 soil samples, MIR reflectance could be measured for 327 samples and vis–NIR reflectance was measured in all 415 samples. Thus, 126 samples had all these three crucial measurements and hence these were used for building the chemometric models; this dataset is called model dataset. The remaining soil samples, called test dataset were used for model evaluation. For the elemental composition, an XRF (Model: AXIOS: PAN Analytical Instrument) equipped with Rh tube was used to analyze major and trace elements. Prior to grinding soils to make <75 μm size fractions by an agate mortar and pestle, each sample was oven dried at 60 °C overnight to remove residual water. Four grams of powdered sample was mixed with 2 g of boric acid powder as the binder and the content was pulverized to mix properly. The mixture was then transferred to an aluminum cup (30 mm) and pellets were prepared using a manual hydraulic press. Pellets were then loaded into the XRF for elemental analysis. Eleven scans were performed in order to cover the X-ray energy of interest. The instrument was set up with a resolution of 10–50 eV to identify the intensity of elements for rich elemental composition. These measurements were performed using helium in the optical chamber of the XRF. Quantitative analyses of spectra were performed using the PAN analytical software OMNIAN, which provides elemental analysis for all type of samples. OMNIAN

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