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Hyper spectral Analysis of Soil Iron Oxide using PLSR Method: A Review

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***Abstract*—** Spectroscopy is a rapid, simple, non-destructive and analytical technique, which provides a good alternative that may be used to replace conventional methods of soil analysis. Soil iron oxides occur in almost all type's soils and they reflect different environmental conditions by the high variability of their mineralogy and concentration. Soil iron oxide, being an important pedogenic indicator of the soil, measurement of Iron Oxide content can be used as an index of soil fertility. Analytical Spectral Device (ASD) Field Spec 4 Spectroradiometer is used which has 350-2500 nm spectral wavelength range to estimate iron oxide content from the soil sample. The Vis-NIR reflectance spectroscopy requires less effort and it is quick innovation to predict the soil iron oxide content. For collecting the soil iron oxide content from spectral data we are utilizing PLSR which is statistical regression method. This paper states the work that is done on different soil types at different places to observe the iron oxide content in soil.

Keywords- *Iron Oxide, Reflectance Spectroscopy, ASD field spec 4, Vis-NIR, PLSR.*

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I. INTRODUCTION

Soils are major elements of land surface ecosystems. Representing these ecosystems and monitoring their changes requires a proper knowledge of the soil development [1]. Soil contains minerals, organic matter, uncountable quantities of organisms and also varying amounts of air and water which gives support to the life [2]. Generally soil fertility is assessed by soil properties such as its contents. Assessment of soil fertility is currently turning into a routine work for soil management and crop production. However, laboratory-analysis based identification of soil properties is time consuming, which is not appropriate for precision agriculture. Here, Reflectance spectroscopy shows up as an option and quick strategy to quantify soil fertility. Iron oxides occur in almost all types of soils and they reflect distinctive natural conditions by the high fluctuation of their mineralogy and concentration [3]. The analysis of iron oxide is of great pedological interest because the iron oxide content in soil reflects the duration and intensity of pedogenesis [4]. Thus this global presence of iron oxides in soils makes them an appropriate pedogenic indicator [5].

Iron oxides form mainly as weathering products of rocks with iron-containing mineralogy, for example, silicates, carbonates, and clays. They present as coatings on other soil particles and act as cementing agents between soil contents. Color is one of the main attribute of soil and iron oxide is one of the main pigmenting agent in soil. Soil colors have been utilized as a part of different studies to survey the iron oxide mineralogy and substance to depict soil advancement and segregate between soils [6]. Spectroscopy in the visible and near-infrared ranges allows rapid acquisition of soil information based on the soil properties [7]. For the analyzation of soil properties, spectral reflectance measurement is a timesaving and non-destructive alternative to traditional methods. It allows a reasonable estimation and is particularly helpful, when large numbers of samples and analyses are required [8].

Reflectance spectroscopy allows soil chemical properties to be determined based on their absorption characteristics. Iron oxide produces wide diagnostic absorption bands in the Visible-Near-infrared region. It is such a promising approach, that it uses diagnostic absorption bands in the reflectance spectrum. These wavelength-dependent properties generate a unique spectral reflectance signature from which materials can be identified and distinguished [9].

Mainly, Reflectance spectroscopy provides the potential to assess various physical, chemical, and biological soil properties and therefore be used as a more efficient technique to determine soil information when rapid, timely analyses are required.

II. SPECTRAL PROPERTIES OF SOIL

Nearly all absorption features in the Visible, NIR and SWIR are overtone or combination bands in the infrared region of the electromagnetic spectrum [10].

Generally properties of soil are distributed in the following way in the VIS -NIR – SWIR region of electromagnetic spectrum:

1. VIS range (400-700 nm) provides a measure of soil color.
2. Broad and shallow absorption bands occur near 500-700 nm are due to oxihydroxides, hydroxides.
3. Narrow and well defined absorptions near 1400 and 1900 nm are related to hydroxyl and water molecules.
4. Absorption features which are beyond 2000 nm are due to clay minerals, organic constituents, carbonates and a wide range of salt minerals.

Different absorptions also occur due to soil constituents throughout the 350-2500 nm range, yet they are hard to determine as they represent weaker tones of soil.

Following is the general spectral signature for iron oxide:

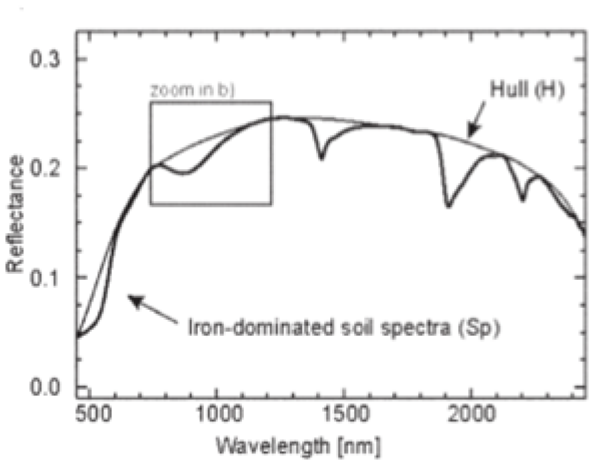

Figure 1. Spectral signature of iron oxide

The wavelengths at which major absorptions because of hematite and goethite occur are close to 880 nm and 920 nm, respectively [11]. However, in some spectra, the presence of iron oxide is difficult to find if iron oxide is present in small amounts or if its absorption is masked by any other content.

III. RELATED WORK

For many years soil analysis has been used as an aid to assessing fertility and quality of soil for plant nutrient management. Achieving and maintaining appropriate levels of soil fertility, especially plant nutrient availability, is of paramount importance if agricultural land is to remain capable of sustaining crop production at an acceptable level. Soil sampling and analysis are equally important steps in managing the nutrients required by plants.

N. Richter et.al., presented a model approach for determining iron oxide in red Mediterranean soils based on the Fe-NIR absorption band and evaluated the spectral influence of variable soil textures on the soil reflectance and Fe-related absorption bands. They showed that the iron oxide absorption bands of clay-dominated soil samples were, in general, deeper than sand dominated samples with comparable iron oxide content. They have evaluated both sample models with low prediction error (sand: $R2v = 0.87$, $RMSEv= 2.72$; clay–silt: $R2v = 0.70$; $RMSEv = 4.13$).

Binny Gopal, Amba Shetty et.al., found that reflectance spectroscopy provides a good alternative that may be used to replace conventional methods of soil analysis. They demonstrated that visible spectroscopy coupled with PLSR can predict topsoil iron oxide with a moderate level of accuracy [12].

Changkun Wang et. al., investigated the potential of visible and near-infrared (Vis-NIR) reflectance spectroscopy for determining Rare Earth elements (REE) in soil. They used Field Spec 4 Hi-Res spectrometer to record soil spectra. Also they used Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) and emission spectrometry (ICP-ES) for the determination of REE. PLSR was used to calibrate the soil spectra and reference values of REE measured by ICP-MS. The result shows that Vis-NIR reflectance spectroscopy provides a feasible method for the simple and rapid determination of REE in soil [13].

Livia Arantes Camargo et.al, demonstrated the importance of diffuse reflectance spectroscopy in estimating clay, iron oxide and adsorbed phosphate contents using a large number of samples. Reflectance values were recorded on a PerkinElmer Lambda950 spectrophotometer equipped within the Visible (VIS) and Near Infrared (NIR) range. They used Partial Least Square Regression (PLSR) within VIS and VIS + NIR ranges. They showed that clay content have higher values of cross-validation parameters within the VIS (with $R2 = 0.80$, $RMSE = 6.89$) and also Hm and Gt have slightly higher values of cross validation parameters within the VIS. They got largest value of the cross-validation R2 for absorbed phosphate within the VIS+NIR range as 0.80 with a RMSE of 46.4mg kg^{-1}. They evaluated the importance of diffuse reflectance spectroscopy in estimating clay, iron oxide and absorbed phosphate. [14].

R. A. Viscarra Rossel et.al., have shown that a VIS–NIR diffuse reflectance spectra can be used to estimate the relative abundance of hematite and goethite in Australian surface soils and derived a Normalized Iron Oxide Difference Index (NIODI) to better discriminate between them. They also derived soil RGB color from the spectra and mapped its distribution and uncertainty across the country using sequential Gaussian simulations. They measured the diffuse reflectance spectra of the soil samples using the Lab spec® VIS–NIR spectrometer with a spectral range of 350–2500 nm. Then spectra were analyzed using principal component analysis (PCA) method [15].

Gladimir V. G. Baranoski et.al., investigated the effects of sand-grain morphology on the visible and near-infrared reflectance of sand soils with different mineralogical characteristics. This investigation was performed using a predictive simulation framework supported by sand characterization data provided in the scientific literature. Using this framework, they performed controlled in silico experiments in which they assessed the interplay between key morphological properties (size, roundness, and sphericity) and mineralogical characteristics (iron-oxide content and particle type distribution) with respect to the spectral signature of sand soils. They found that the influence of grain morphology may vary considerably depending on the distribution patterns of iron oxides present in sand-textured soils [16].

T. J. Cudahy, E. R. Ramanaidou et.al., found that field spectral method is accurate for measuring the hematite-goethite ratio compared with the laboratory-based methods. They demonstrated that the hematite-goethite ratio of ooidal iron deposits can be measured in the field using VNIR spectrometry [17].

Joanna E. Bullard, Kevin White et. al., studied a rapid technique for quantifying ‘‘redness’’ in the field using visible reflectance spectrometry. They demonstrated the relationship between increasing redness and increasing concentrations of iron oxide in the sediments is strong and positive. The result shows that simple field spectral measurements are able to provide reliable estimates of iron oxide concentrations and redness, therefore negating the need for more detailed controlled laboratory measurements [18].

Angelica Santos et. al., have evaluated what are the procedures to estimate of iron oxides in soil more accurate, fast and economical for the mapping of large areas, with potential use in pedometrics. They have compared the traditional technique (x-ray diffraction) with indirect method (diffuse reflectance spectroscopy). They found that DRS in the visible and near infrared (Vis-NIR) is a good alternative to laboratory analysis of physical, chemical and mineralogical attributes [19].

Renato Eleoterio de Aquino et. al., showed that the color as measured by diffuse reflectance spectroscopy proved efficient to indicate variations between the Archeological Dark Earth, proving to be an innovative technique, efficient and promising for indirect quantification of soil attributes in a simple manner. Also they found that iron oxides are sensitive indicators of pedoenvironmental and pedogenic processes of Archeological Dark Earth. According to authors, Hematite and goethite minerals determined by x-ray diffraction and diffuse reflectance spectroscopy, besides not presenting significant variations between the soils, have similar characteristics to non-anthropogenic Brazilian soils. They used PCA method to evaluate the interaction of physical, chemical and mineralogical attributes [20].

V.M. Sellitto et.al., compared two different spectroscopic techniques for the characterization of soil iron oxides, diffuse and bi-directional reflectance. The result shows that soil spectra, either from Bi-Directional Reflectance (BDRS) and Diffuse Reflectance spectroscopy (DRS), enable the detection of small amount of hematite and goethite across the VIS-NIR region that provides information regarding the iron oxide minerals content. In this, Diffuse Reflectance (DR) spectra were recorded from 380 to 900 nm using a Varian Cary1E spectrophotometer and Bi-directional reflectance was measured in the laboratory under artificial light, using an ASD Field Spec Pro 350–2500 nm spectroradiometer. Their goal was to compare the reflectance measurements on air dry soil obtained by both a spectrophotometer and spectroradiometer under laboratory conditions [21].

Eileen Eckmeier, Renate Gerlach et.al., states that VIS spectra can be used as an analytical tool. They used spectral information to build predictive models from the measured VIS spectra of sample sets with known properties (laboratory analysis) based on Partial Least Squares Regression (PLSR).The result shows that the presence of charcoal highly correlated with the lightness of soils, while in the samples with lower concentrations of organic matter and high contents of $CaCO_3$, the presence of iron oxides and carbonates mediated soil colors [22].

Monika Hanesch et.al., studied Raman spectroscopy of synthetic and natural iron (oxy) hydroxides and iron oxides to test its potential in environmental magnetic studies and soil science. Their main aim was to distinguish between the different iron oxides occurring in soils [23].

Shengxiang Xu et al, demonstrates the importance of a practical subsetting strategy for the continued improvement of Soil Organic Matter prediction with Vis–NIR spectroscopy. They used Field spec 4 spectroradiometer to record diffuse reflectance spectra in the Vis–NIR (350–2500 nm) range. Also they used PLSR method to correlate the spectral data with laboratory SOM measurements [24].

Ashwini Dilip Padmanabhi, Dr. R. R. Deshmukh et.al., have done research on Vis-NIR reflectance spectroscopy to calculate soil Nitrogen content. They used Analytical Spectral Device (ASD) Field Spec 4 Spectroradiometer which has 350-2500 nm spectral wavelength to identify total nitrogen content from the different soil sample. They utilized Partial Least Square Regression (PLSR) technique for feature extraction of soil spectral signature [25].

Dnyaneshwar D. Karale, Dr. Ratnadeep R. Deshmukh et.al., treated visible and near Infrared (Vis-NIR) reflectance spectroscopy as a strategy with fast and minimal effort to determine Soil Organic Carbon (SOC) content. The research indicates that the importance of a practical strategy for the improvement of Soil Organic Carbon (SOC) prediction with Vis–NIR spectroscopy. They used PLSR regression model to estimate the carbon content in the soil [26].

Richard J. Murphy et.al., studied that determination of wavelength position of absorption features in the VNIR (400–1200 nm) from hyper spectral imagery is more challenging than that for data acquired using non-imaging instruments. The conclusion of this study is that the wavelength position of features in the VNIR should be determined from imagery using a polynomial (or equivalent) fit to the data and not from the original data themselves [27].

Snehal N. Kulkarni, Dr. Ratnadeep R. Deshmukh et.al., have evaluated Carbon, Nitrogen, Phosphor and Water Contents from Agricultural Soil by Reflectance Spectroscopy using ASD Field spec Spectroradiometer. The objective of their paper was to know the suitability and sustainability of soil, to make soil fertilizer for improving the soil quality. The soil spectral signatures were taken by ASD spectroradiometer and they compare those for different soil samples. They have discovered carbon, nitrogen, phosphor and water contents of soil and they also compared different soil samples of Aurangabad district using Principle Component Analysis (PCA) [28].

Marco nocita et. al., have done research on soil spectroscopy as a tool to survey organic carbon, iron oxides, and clay content in the subtropical thicket biome. They present a project dealing with organic carbon, iron oxides, and clay content assessment, in the degraded thicket biome, through the combination of soil spectroscopy and Partial Least Square Regression (PLSR) techniques. The soil samples have been chemically and spectrally analyzed. The study models the relationships between soil spectral reflectance’s, measured in situ and in the laboratory, and the soil parameters taken in consideration. They have been analyzed topsoil samples with and without stones, in order to determine the influence of the stone Layer on the soil spectral reflectance, as assessed with the field spectrometer, while the 0-20cm soil samples have been analyzed without stones. The result shows that soil stoniness is an important variables to consider for the soil

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properties prediction models creation. They developed PLSR model with laboratory and field spectra offered very good results for the prediction of SOC (calibration and validation r2> 0.7, rmsev<0.6), and mediocre results for the iron oxide prediction (rmsev always >0.55).The clay content prediction models production is at a preliminary stage [29].

IV. Field Spec Spectroradiometer

The measurement of spectral reflectance in the laboratory using FieldSpec spectroradiometer allows us to study on specific influences on the reflectance under controlled conditions. FieldSpec spectroradiometer is used to identify soil properties and its contents for proper soil management [30].

The instrument has following specifications:
1. Spectral Range- 350to 2500nm
2. Rsolution-3nm (at 700nm) to 10nm (at 1400 and 2100nm)
3. Bandwidth (Spectral sampling)-1.4nm @350-1000nm and 2nm @ 1000-2500nm
4. Bands-2151

For sample measurement using FieldSpec spectroradiometer, it requires air-dried samples. Halogen light source is used as an illumination. To collect incident light on sample, fibre optic cable is used which has a 25° Field Of View (FOV). By using RS3 software in laptop we can acquire spectra of samples.

Following is the setting structure of the ASD spectroradiometer:

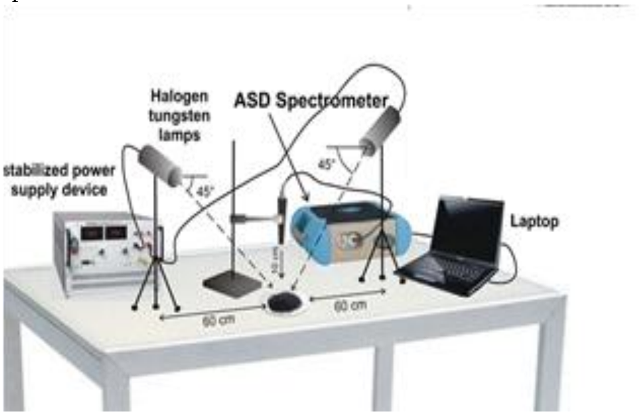

Figure 2. Setting and the internal structure of the ASD spectroradiometer [31]

V. Conclusion

The above study shows that there are many different methods to detect soil iron oxide using remote sensing and GIS, so either by using reflectance spectroscopy or traditional methods it is possible to detect iron oxide in soil. Among these methods, Reflectance spectroscopy brings a good alternative which may be used to alter traditional methods of soil analysis. In spectroscopy the characterization of content is depend upon the obtained reflectance. Hence spectroscopy is suitable method to analyse the soil iron oxide content. Many of the authors used different methods such as Principle Component Analysis (PCA) and Partial Least Square Regression (PLSR) to relate spectral reflectance with measured properties of samples. But PLSR is considered as a robust technique which deals with colinearity of predictor variables and accounts for both the x and y variable to estimate soil property.

So from the above study, we found that visible and Near-infrared reflectance spectroscopy is a rapid and non-destructive analytical technique which requires little sample pre-treatment and has been successfully used to determine soil properties.

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