

MULTI-TEMPORAL PREDICTION OF CONTAMINATING MINERAL ABUNDANCE USING HYPERSPECTRAL SPECTROSCOPY

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ABSTRACT

Mine tailings, charged with toxic minerals, of the abandoned mining of Hammam Zriba in the north of Tunisia are continually exposed to erosion and thus destroys the normal function of soils and endangers human health. Characterization, estimate and efficient monitoring of the abundance of minerals with high pollution potential in a quick and timely fashion is crucial for protecting the natural environment. Particularly, detecting changes in abundance of mineral concentrations measured in the same collection points at different time series is of special interest in this application domain. In this context, field Hyperspectral spectroscopy and X-ray diffraction (XRD) method were used to characterize of both several minerals. The partial least squares regression (PLSR) method was processed for the prediction of mineral contents.

Index Terms—Hyperspectral field spectroscopy, PLSR, Mine tailings, Change detection.

1. INTRODUCTION

Mining activity are sources of soils vegetation and water pollution with heavy metals in many parts of the world [1]; [2]. However, significant quantities of mining waste, charged by heavy metals such as Pb, Zn, Cd etc, and minerals with high pollution potential (Ba and F), have a wide spread distribution [2]. Thus, monitoring the environmental risks associated with mine wastes in a quick and timely fashion is the first step towards mitigating their impact. Several previous studies have proven the efficiency of the PLSR method for the prediction of existing minerals, including minerals with high pollution potential which do not have an absorption feature, within soils from their visible, near-infrared (VNIR) and short-wave infrared (SWIR) laboratory and field hyperspectral spectra [3]; [4]; [5].

Our contribution consists in the characterization of both several minerals, including minerals with high pollution potential, content within agricultural soils from and change detection of abundance. We are particularly interest in detecting changes in abundance of minerals measured at different time instants of the same collection points using field Hyperspectral spectroscopy with respect to XRD analysis.

The PLSR method was processed for a predicted the minerals contents within agricultural soils around Hammam Zriba mine site in the North of Tunisia. The case study of Fluorite and Barite, which is forsaken since 1992, is located near the village of Hammam Zriba, the olive groves and the Oued El Hammam [2]; [4]. In this site, a volume of 260,374 m³ of tailings which were stored in three dikes between 5 and 10 m of high.

2. METHODOLOGY

The methodology proposed in this study was applied using field VNIR-SWIR spectra measured in the same collection points at two dates (March 2017 [4]; [5] and March 2016).

In March 2016, a total of fifty-four soil samples were accurately located using DGPS and collected from the surface layer (0–5 cm). Soil samples were particularly, collected around dikes, according to the sensitivity of certain areas such as olive fields, areas exposed to wind and water erosion, and areas of low slope. All soil samples were analyzed by XRD method for the identification of their mineralogical composition as well as their abundances. Hyperspectral measurements of wastes and soil were measured on the field on the same 54 collection points, under natural light (sun), using an Analytical Spectral Device ASD Spectrometer HiRes4. This spectral analytical device provides information between VNIR-SWIR (350–2500 nm). The number of spectral bands was reduced to 1775, instead of 2151 bands, by removing the spectral regions between 350–399 nm, 1350–1450 nm, 1820–1950 nm and 2401–2500 nm.

A PLSR method was used to model relationship between mineral contents obtained from XRD analysis and the measured reflectance spectra of samples. Mineral concentrations are sorted in increasing and decreasing order to explore the difference related to the division of the whole dataset into calibration and validation sets. After sorting the mineral concentrations, 25% of the samples were dedicated to validating the PLSR model and 75% of the samples were used for model calibration purposes. Where the first sample was put in a validation set and the next three samples are put in the calibrations set. Then the procedure is continued for all the samples by alternately placing the following in the validation set and the next three samples in the calibration set. The maximum number of latent variables in the PLSR was defined as 15. Once each PLSR model was built using the Cross-validation dataset. The prediction performance of the PLSR models was evaluated using: the coefficient of determination R^2 , the root mean square errors of cross-validation (RMSECV), the root mean square errors in the validation set (RMSEP), the ratio of performance to deviation in the validation set (RPD), the RMSEP and the ratio of the performance to interquartile (RPIQ) [4].

3. RESULTS AND DISCUSSIONS

3.1. Mineralogical and spectral characterization of soil samples

The XRD analysis results (Figure 2) revealed a predominance of calcite, barite, fluorite and quartz. Less important abundances was however, indicated by sphalerite and kaolinite. Clays was detected particularly in the soil samples with low concentrations. Hemimorphite, smithsonite, pyrite and galena are however rarely detected within dykes and at nearby soils as well. According to these results, both fluorite and barite constitute the principal minerals that cause pollution. The laboratory results indicated a difference of the concentrations between 2016 and 2017, especially the concentrations of barite, sphalerite, calcite and hemimorphite were also higher in 2017 compared to 2016 (Figure 2). The results can be explained by the quantities of tailings that were transported by the hydrous and eolian erosions.

The absorption peak identified in SWIR region at 2340 nm (Figure 1) is associated with CO_3 overtone vibrations, confirms the presence of carbonates and particularly the calcite (CaCO_3) mineral in this site [6].

Another absorption peak is identified at 2206-2208 nm, especially in the soil spectra (Figure 1). It is a characteristic absorption due to the combination of OH-Al bending and OH stretching modes associated with the presence of clays [7]; [8]. Quartz, Fluorite and Barite minerals cannot be observed in VNIR-SWIR regions, as they do not have a specific absorption feature [4]; [5].

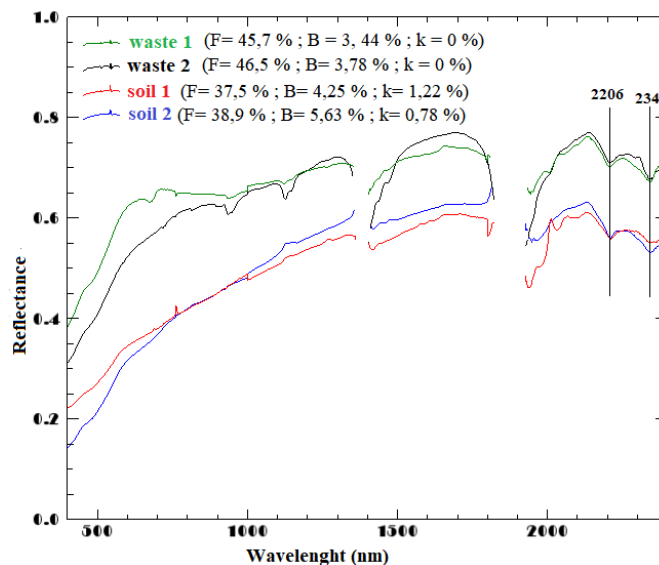


Figure 1: Plot of the VNIR-SWIR spectral profiles of mine wastes and soil samples measured in (1) 2016 and (2) 2017.

3.2. Prediction results of the PLSR models

PLSR model performance statistics using VNIR-SWIR reflectance spectroscopy, measured in Marsh 2016, and minerals concentrations revealed by the XRD analysis were calculated and shown in Table 1.

Compared to the VIP scores and the b-coefficients for the VNIR-SWIR reflectance measured in Marsh 2017 [4]; [5], the same absorption feature band for both Fluorite and Barite predictions. Particularly, absorption feature band at around 2206 nm, caused by the combination of OH-Al bending and OH stretching modes, related to the presence of clays [7], seems to be useful for the estimation of fluorite and barite contents.

Considering the concentrations in increasing order, the highest prediction accuracies were obtained for the fluorite contents prediction model with an R^2_{cv} superior to 0.62, an RPD_{cv} around 1.38, an R^2_{val} superior to 0.52 and an RPD_{val} around 1.5. The results of the barite prediction model are also interesting and display an R^2_{cv} of 0.65, an RPD_{cv} around 1.47, an R^2_{val} of 0.74 and an RPD_{val} around 2.05. The PLSR model for quartz content prediction has an R^2 and RPD in the calibration set reached 0.7 and 1.65, whereas in the validation set, they are at 0.56 and 1.56, respectively. A satisfied result was showed for kaolinite and display an R^2_{cv} of 0.66, RPD_{cv} = 1.56, R^2_{val} of 0.68 and RPD_{val} = 1.84. Besides of fluorite, barite, kaolinite and quartz almost of the others calcite, hemimorphite and sphalerite minerals gave RPD values under 1.40 and $R^2 < 0.5$ in the calibration and validation sets (table 1).

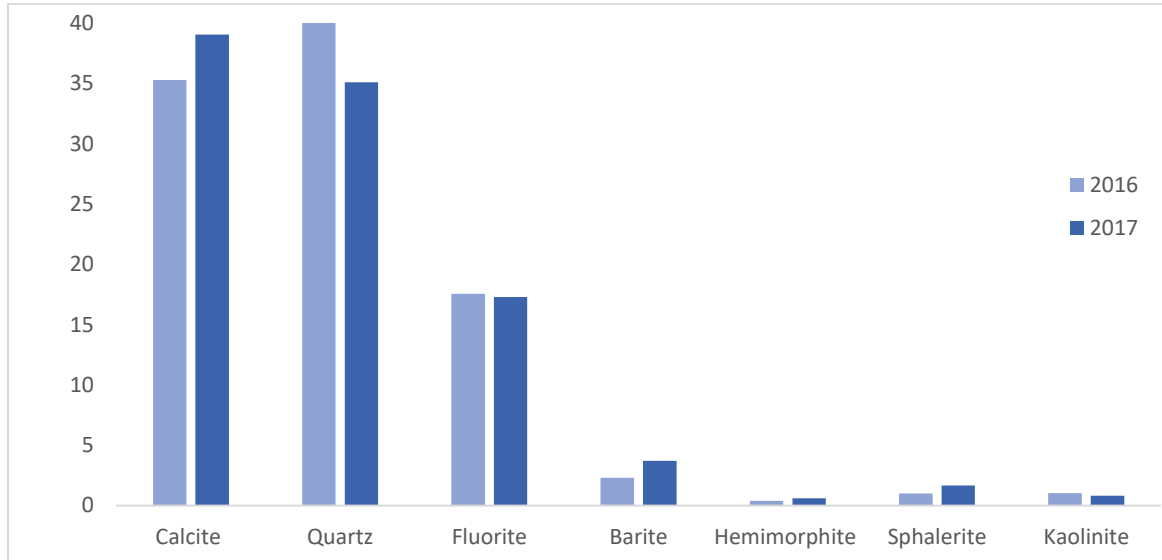


Figure 2: Comparison of the abundance of minerals, between 2016 and 2017, revealed by XRD analysis results (%).

Table 1: Prediction results of the PLSR models obtained from the VNIR-SWIR reflectance (400–2400 nm) and considering the mineral concentrations in both increasing and decreasing order.

		Calibration set (75% data)				Validation set (25% data)					LV
Element (%)		n	R ² _{CV}	RMSECV	RPD _{cv}	n	R ² _{val}	RMSEP	RPD _{val}	RPIQ _{val}	
Increasing order	Barite	39	0.65	1.31	1.47	13	0.74	1.08	2.05	3.26	3
	Calcite	39	0.15	9.99	0.66	13	0.26	7.53	1.21	1.34	3
	Fluorite	41	0.62	11.09	1.38	13	0.52	12.21	1.5	2.69	3
	Sphalerite	39	0.56	1.03	1.21	13	0.05	1.03	1.04	1.21	2
	Hemimorphite	38	0.28	0.53	0.73	13	0.3	0.53	1.24	1.34	2
	Quartz	40	0.7	12.45	1.65	13	0.56	14.12	1.56	2.6	3
	Kaolinite	40	0.66	0.57	1.56	13	0.68	0.45	1.84	2.96	3
Decreasing order	Barite	39	0.71	1.2	1.64	13	0.64	1.2	1.56	2.88	3
	Calcite	40	0.27	9	0.79	13	-0.13	9	0.54	0.86	3
	Fluorite	40	0.6	11.25	1.33	13	0.61	11.25	1.52	2.71	3
	Sphalerite	40	0.51	1.06	1.08	13	0.59	1.06	1.5	2.7	2
	Hemimorphite	40	0.31	0.51	0.94	13	0.2	0.51	1.18	1.30	5
	Quartz	40	0.66	13.26	1.59	13	0.56	13.26	1.47	2.6	7
	Kaolinite	39	0.69	0.51	1.79	13	0.58	0.51	1.50	2.7	12

n: number of samples.

Considering the mineral concentrations in decreasing order, results (table 1) have shown an accurate prediction of the same fluorite ($R^2_{cv}=0.6$ and $RPD_{cv} = 1.33$; R^2_{val} of 0.61 and $RPD_{val} = 1.52$), barite ($R^2_{cv}=0.71$ and $RPD_{cv} = 1.64$; R^2_{val} of

0.64 and $RPD_{val} = 1.56$) and kaolinite ($R^2_{cv}=0.69$ and $RPD_{cv} = 1.79$; R^2_{val} of 0.58 and $RPD_{val} = 1.50$) into calibration and validation sets. Also, the sphalerite model shows highest R^2_{val} and RPD_{val} at 0.59 and 1.5, respectively, for validation

results. It's shown in this study compared to previous ounces [4]; [5], that an inaccurate prediction model was obtained for calcite mineral (table 1) despite its higher concentrations within both soils and mine tailings.

A variation in the accuracy of prediction (R^2 and RPD values) was showed between Marsh 2017 [4]; [5] and Marsh 2016. The change in the accuracy of prediction shows the differences in the concentrations of minerals between 2016 and 2017. The effects of water and wind erosion are almost shown in this part. It can be seen that a large amount of waste was changed in the one year.

4. CONCLUSION

These results show that PLSR regression method using VNIR/SWIR reflectance spectroscopy, is promising for risk mineral contents estimation, which do not have an absorption feature. This study presents a considerable contribution in the identification of changed in abundance of mineral concentrations during this one year.

5. REFERENCES

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