

Visible and near infrared reflectance spectroscopy for field-scale assessment of Stagnosols properties

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ABSTRACT

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Spectral data contain information on soil organic and mineral composition, which can be useful for soil quality monitoring. The objective of research was to evaluate hyperspectral visible and near infrared reflectance (VNIR) spectroscopy for field-scale prediction of soil properties and assessment of factors affecting soil spectra. Two hundred soil samples taken from the experiment field (soil depth: 30 cm; sampling grid: 15 × 15 m) were scanned using portable spectroradiometer (350–1050 nm) to identify spectral differences of soil treated with ten different rates of mineral nitrogen (N) fertilizer (0–300 kg N/ha). Principal component analysis revealed distinction between higher- and lower-N level treatments conditioned by differences in soil pH, texture and soil organic matter (SOM) composition. Partial least square regression resulted in very strong correlation and low root mean square error (RMSE) between predicted and measured values for the calibration (C) and validation (V) dataset, respectively (SOM, %: $R_C^2 = 0.75$ and $R_V^2 = 0.74$; $RMSE_C = 0.334$ and $RMSE_V = 0.346$; soil pH: $R_C^2 = 0.78$ and $R_V^2 = 0.62$; $RMSE_C = 0.448$ and $RMSE_V = 0.591$). Results indicated that hyperspectral VNIR spectroscopy is an efficient method for measurement of soil functional attributes within precision farming framework.

Keywords: nitrogen fertilization; remote sensing; non-destructive method; climatic condition; soil texture; linear calibration

Soil organic and mineral compounds can be estimated non-destructively by visible and near infrared reflectance (VNIR) of electromagnetic radiation from the surface of the sample, allowing more intensive sampling, reducing the number of expensive laboratory or field assessments and estimating several soil properties from one reflectance curve (Sørensen and Dalsgaard 2005). However, there is a need to supplement soil spectral databases with new calibrations associated with diverse soil conditions, which will be validated to test the impact of soil heterogeneity on spectral algorithms and wavelengths used for the specific prediction. Due to broad and overlapping absorption of soil constituents, VNIR soil spectra is largely nonspecific and results in complex absorption patterns. Absorptions in the visible region (400–760 nm)

are primarily associated with minerals that contain iron and darkness of soil organic matter (SOM) (Stenberg et al. 2010). Visible region was found to significantly contribute to the overall absorption due to SOM (Islam et al. 2003, Viscarra Rossel et al. 2006). Climatic and drainage conditions each have a significant influence on soil colour and further complicate the relation between spectral response and SOM (Stoner and Baumgardner 1981). Soil pH is reflected in complex spectral response due to its covariation with several spectrally active soil properties such as the presence of clay minerals, buffering capacity of SOM and microbial processes in the soil (Chang et al. 2001). Soil texture affects reflectance, as incoming radiation is scattered differently by coarse particles as compared to fine particles. If the particles are more compacted due to the finer

texture, spectral response is intensified because of the higher absorption surface and stronger reflection. Demattê et al. (2004) adopted a descriptive approach using a spectral reflectance-based strategy to assist soil survey and found that SOM, total iron, and mineralogy were the most important attributes influencing reflectance intensity, and allowed characterization of soils. Viscarra Rossel et al. (2011) showed that VNIR reflectance spectra can replace the use of traditional soil properties to describe the soil and make pedological interpretations of its spatial distribution.

The research goal was to evaluate the ability of VNIR spectroscopy for assessment of soil properties in terms of variable mineral nitrogen (N) fertilization and intensive crop production. The objectives included: (a) determination of factors affecting soil spectral properties; (b) discrimination of different N fertilization treatments based on soil spectra; (c) farm-scale prediction of SOM content and soil pH.

MATERIAL AND METHODS

Experimental design and soil sampling. The research was conducted on the experimental field within hydro-ameliorated cropland in the Western Pannonia subregion of Croatia (45°33'N, 16°31'E). It was established as a non-randomized block design of ten different mineral N fertilization treatments with uniform phosphorus (P) and potassium (K) fertilization rates (I. Control – no fertilization; II. N₀PK; III. N₁₀₀PK; IV. N₁₅₀PK; V. N₂₀₀PK; VI. N₂₅₀PK; VII. N₂₅₀PK + phosphogypsum; VIII. N₂₅₀PK + dolomite; IX. N₃₀₀PK; X. fallow, kg N/ha) and four repetition plots for each treatment (1–4). Dimension of each treatment plot was 30 × 130 m including blank space, and 26 × 26 m for the repetition plot, with the total experimental area of 4 ha. Basic fertilization for winter wheat (*Triticum aestivum* L.) as a test crop during the vegetation period 2009/2010, in form

of 2:3 of the total amount of PK mineral fertilizer, was applied before ploughing, while other 1:3 of the total amount with 30% of N was applied directly before seedbed preparation. In all treatments except control, soil was treated with 150 kg P and 100 kg K, in form of triple superphosphate, 60% potassium chloride and complex mineral fertilizer NPK 10-30-20. Nitrogen topdressing was performed three times using calcium ammonium nitrate (CAN): I. 25%; II. 25% and III. 20%. Semi-automatic circular tractor soil probe prototype (Patent: International Application No. PCT/HR2011/000021) was used for sample collection after harvest (20 July, 2010) with total number of 200 soil samples taken at 30 cm depth (regular grid: 15 × 15 m), meaning 20 samples per treatment and 5 samples per repetition plot. Each sampling location was precisely defined (± 1 cm) using GPS (Trimble GNSS R8, Sunnyvale, USA). The point sampling scheme was a circular line sampling of 0.5 m radius around the grid node representing the sampling site of the 16-samples soil composite.

Agroecological conditions. Based on the rainfall amount of the vegetation period 2009/2010 (850.7 mm) and comparison with the reference period 1965–1990 (699.3 mm), the investigated period can be found as sufficiently wet. Soil type of the trial site is classified as Dystric Stagnosols (IUSS Working Group WRB 2015). Terrain is flat with average elevation of 97.2 m a.s.l. Based on the soil profile analysis, soil texture of arable topsoil was defined as loam. Precipitation water periodically stagnates on illuvial horizon which was the reason for installing a pipeline drainage system across the experimental area. Besides soil physical properties that influence water stagnation in upper layers, main factors that limit crop yield are low soil pH and very low SOM content (Table 1). Figure 1 shows within-field spatial variability of soil pH, SOM content and total N content (0–30 cm depth) measured in 2010 after winter wheat harvest (ordinary kriging) (ArcView, ESRI 2006). A sequence of changes in pH values was influenced

Table 1. Soil chemical and physical properties (adopted from Mesic et al. 2011)

Depth (cm)	pH _{KCl}	SOM (%)	Nutrient amount (mg/100 g)		Soil particles (ø mm, %)				Soil texture	Porosity		Water capacity		Air capacity	
			P	K	2–0.2	0.2–0.02	0.02–0.002	< 0.002		vol. %	qualifier	vol. %	qualifier	vol. %	qualifier
0–30	4.84	1.01	7.73	8.67	0.36	55.24	30.30	14.10	loam	43.7	low	39.7	medium	4.0	very low

SOM – soil organic matter

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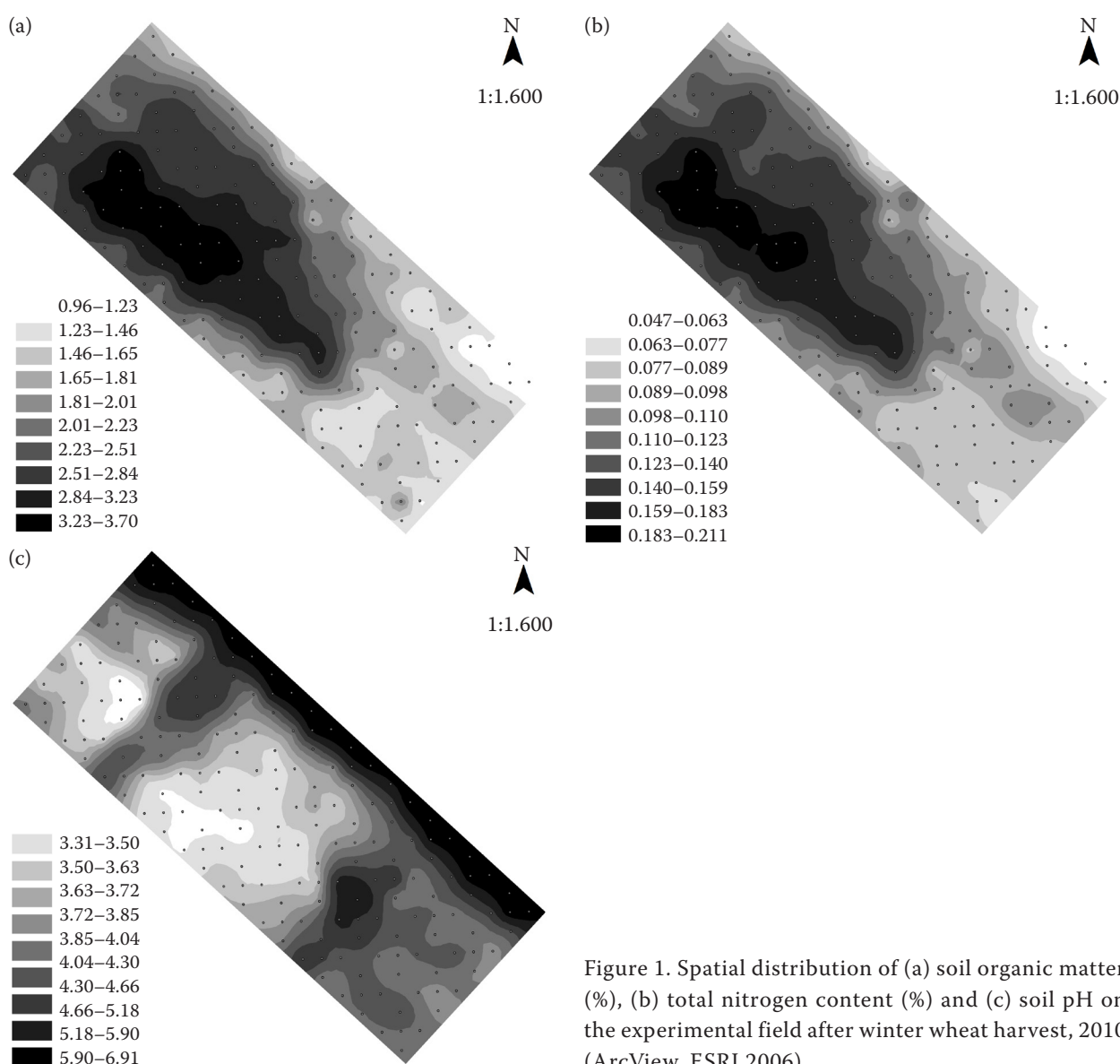


Figure 1. Spatial distribution of (a) soil organic matter (%), (b) total nitrogen content (%) and (c) soil pH on the experimental field after winter wheat harvest, 2010 (ArcView, ESRI 2006)

by increasing N mineral rates, influence of lime materials on treatment VIII, effect of parent substrate in treatment with 100 kg N/ha as a result of drainage, and canal deposit on the north-eastern side of field. According to the increasing N rates and higher crop yields during the experimental years, the highest content of SOM and TN was

recorded in treatments with 250–300 kg N/ha. Relations between soil pH, SOM and total N content were calculated and presented in the correlation matrix with strong to full significant correlations between variables (Table 2).

Spectral measurements. Non-destructive measurements of soil reflectance were performed using

Table 2. Correlation matrix between different soil properties ($n = 200$)

Variable	Mean	Standard deviation	pH	TN (%)	SOM (%)
pH	4.404	0.962	1.000	–0.574	–0.523
Total nitrogen (TN, %)	0.122	0.037	–0.574	1.000	0.983
Soil organic matter (SOM, %)	2.189	0.674	–0.523	0.983	1.000

Correlations are significant at $P < 0.05$

a portable field spectroradiometer (FieldSpec®3, ASD Inc., Boulder, USA) with a wavelength range from 350 nm to 1050 nm, sampling interval of 1.4 nm and spectral resolution of 3 nm at 700 nm. Air-dried samples were milled and passed through the sieve (< 2 mm), placed on 9-cm diameter Petri dishes (borosilicate glass) forming 1.5-cm soil layer. Two hundred soil samples were scanned under laboratory conditions at fixed distance of 1 cm using a vertically positioned hand-held fiber-optic probe. Calibration panel (Spectralon®, Labsphere, North Sutton, USA) measurements were taken before initial soil readings and repeated approximately every 15 min.

Laboratory measurements. Standard laboratory analyses were used as reference measurements for calibrating spectral data. Air-dried soil samples ($T < 40^{\circ}\text{C}$) were crumbled, sieved (< 2 mm), and homogenized following the ISO 11464 (2004). Soil pH was measured in a 1:2.5 (w/v) soil suspension [1 mol/L KCl, modified ISO 10390 (2005)]. Total nitrogen content (TN [% DM; g/kg]) and total carbon content (TC [% DM; g/kg]) in soil were determined by dry combustion method according to HRN ISO 13878 (2004) and HRN ISO 10694 (2004), respectively. Regarding very low average soil pH indicating acid soil, and assumption that mineral carbon is not present in investigated soil, TC can be equalized to soil organic carbon. In that manner, SOM was calculated from the TC content multiplied by the Van Bemmelen factor 1.724.

Statistical analysis. Spectral data were visually evaluated using the ViewSpec Pro 4.07 (2009). Original reflectance data (700 wavelengths) were calibrated to the SOM content and soil pH by partial least squares regression (PLSR) and full cross validation (Unscrambler 9.7, 2007). Statistical parameters used for the model accuracy included coefficient of determination (R^2) and root mean square error (RMSE) with confidence limits of 95%.

RESULTS AND DISCUSSION

Treatment effect on soil reflectance. Different N fertilization rates indicated similar soil spectral response, but with certain variations of reflectance intensity appearing throughout the spectral range (Figure 2). The pattern of spectral reflectance was calculated: higher SOM content-lower reflectance, and contrary, lower SOM-higher reflectance. Lower soil reflectance at treatments N_{100}PK , fallow,

N_{250}PK , $\text{N}_{250}\text{PK} + \text{phospho-gypsum}$ and N_{300}PK can be explained by higher SOM content due to more intensive mineral fertilization (Figure 1), shorter period for SOM decomposition process, higher microbial activity and crop residue amount due to greater biomass. Despite numerous absorption bands of organic matter over the VNIR region, it is often reported that organic matter signals in this region are weak (Viscarra Rossel and McBratney 1998), particularly in soils that contain only a few percent organic matter (as 1.0–3.7% at this experimental site), in a variable mineral matrix. Low reflectance curve concavity and weaker absorption can be observed around 450 nm and 850 nm. Due to the eluvial process, it can be assumed that clay and free iron oxides were been removed, or segregated to the extent that colour of the horizon is determined by colour of sand and silt particles, which caused high reflectance intensity throughout the whole spectrum (average reflectance factor: 0.55–0.60). Natural renewal of SOM affected soil reflectance at the fallow treatment considering that this treatment was ploughed but not sowed. In the spectral range of 490–560 nm, spectral response confirmed conclusions given by McCoy (2005) about lower soil reflection where higher presence of SOM, total N and lower soil pH were recorded. In this case, lower level of mineralization indirectly affected decreased SOM decomposition. Similar results were reported by López-Granados et al. (2005) who found that high-SOM areas correlated with low-pH zones probably due to the presence of organic acids and unsaturated acidic humus.

Partial least squares regression. Considering the results of a correlation analysis between soil properties, PLSR for SOM was calculated based on the spectral data. Regression model for soil pH was calculated to find indirect relations with SOM and the potential outliers in the data. Figure 3 shows the results of the PLSR model calibrated to estimate SOM content (upper figure) and soil pH (bottom figure) using original soil reflectance (700 wavelengths across full spectral range of 350–1050 nm) and reference sample data (200 samples). The score plot gave information about patterns in the samples in terms of delineation between higher and lower SOM content in soil samples based on the reflectance data. As seen for soil pH, low values prevailed based on the principal component (PC) scores. First two components for

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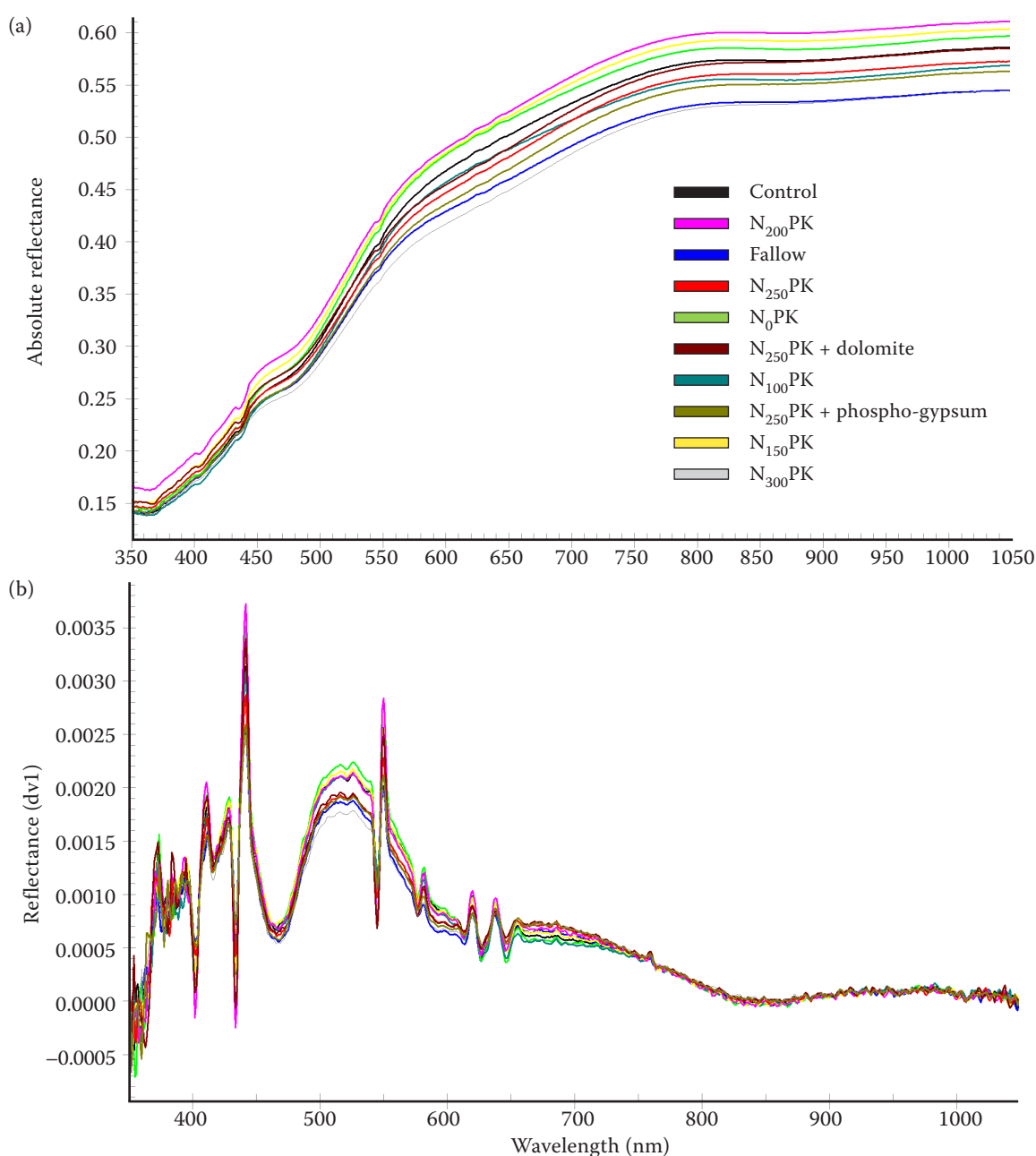


Figure 2. (a) Average absolute reflectance and (b) average first derivative of soil reflectance (dv1) at ten fertilization treatments

both SOM and soil pH summarized the most variation in the data captured by VNIR spectra (PC1: 94%, PC2: 4% and PC1: 93%, PC2: 6%, respectively). As seen from the regression coefficients plot, red part of the spectrum (670–710 nm) with red edge region (730–770 nm) were identified as zones of major importance for the PLSR model of SOM content. Nanni and Demattè (2006) recorded spectral ranges of 480–600 nm and 720–820 nm as key regions for SOM prediction model development. Regarding the residuals of soil pH prediction, exclusion of several

outliers could improve prediction and decrease residual variation. According to the PLSR statistics, a very strong correlation and low RMSE were obtained between predicted and measured values for the calibration (C) and validation (V) dataset, respectively (SOM, %: $R_C^2 = 0.75$ and $R_V^2 = 0.74$, $RMSE_C = 0.334$ and $RMSE_V = 0.346$; soil pH: $R_C^2 = 0.78$ and $R_V^2 = 0.62$, $RMSE_C = 0.448$ and $RMSE_V = 0.591$), as shown in the scatter plot right below in each figure. Prediction scores of soil pH formed two groups of distribution. Small formation of scores (right) rep-

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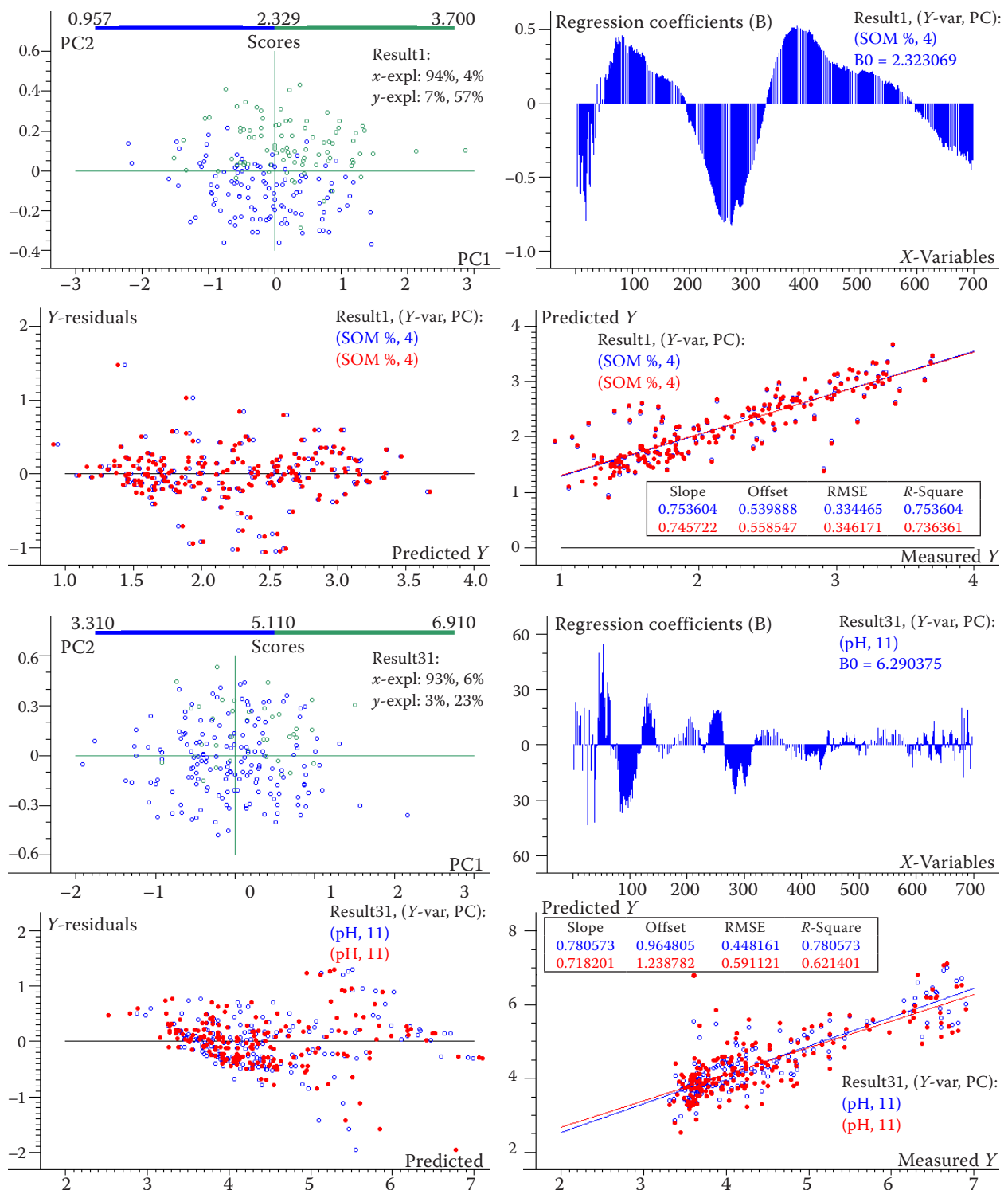


Figure 3. Scatter plots for results of the partial least squares regression (PLSR) model performed using full cross-validation method from soil reflectance data showing a relationship between predicted and observed soil organic matter (SOM) content (%) (upper plot) and soil pH (lower plot) ($n = 200$). \circ – calibration; \bullet – validation; RMSE – root mean square error

resents samples with higher soil pH values, while larger 'cloud' on the right side of the regression trend line represents prevailing values of low soil

pH. Very similar results were reported by Zhang et al. (2011) where R^2 for SOM validation model was 0.764 (particle size of air-dried soil sample < 0.15 mm)

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and $RMSE_V$ was 0.344. Qiao et al. (2017) used PLSR for SOM prediction based on hyperspectral data with different preprocessing methods. Their statistics of calibration ($n = 165$) and validation ($n = 55$) results are comparable with this research ($R^2 = 0.83$ and $R^2 = 0.61$, $RMSE_C = 0.266$ and $RMSE_V = 0.419$). VNIR spectroscopy predictions using PLSR models and cross-validation were considered reliable for SOC ($R^2 > 0.80$), and SOM ($R^2 = 0.83$), based on the results of Luce et al. (2014) and Feyziyev et al. (2016), respectively. Regarding the soil pH predictions, reviewed literature reports reliable calibrations on a field-scale due to site-specific covariations of soil pH to other soil fertility variables, with $RMSE$ values between 0.19 and 0.31 and R^2 values between 0.53 and 0.73 (McCarty and Reeves 2006, Viscarra Rossel et al. 2006).

According to the results of this research, a model obtained by PC explanatory analysis and PLSR was able to integrate pedological information from a number of spectral bands for estimating SOM content and soil pH, and to reveal delineation between higher- and lower-N level treatments conditioned by differences in soil properties. Regarding further work, more distinct information may be obtained using the instruments with a wider spectral range covering NIR and shortwave infrared radiation, where more apparent soil absorption features could be recorded and used for monitoring of soil functional attributes and making inferences about its quality.

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