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# Visible and near-infrared spectroscopy in Poland: from the beginning to the Polish Soil Spectral Library

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**Abstract.** Worldwide, there is a growing interest in the use of visible and near-infrared spectroscopy (VIS-NIRS) to characterise soils. The method is largely used in the agricultural (foods and cereals) sector but is only in the research phase for soil analysis despite the fact that it is a suitable tool for precision agriculture. A quick search at the Web of Science (WoS) Core Collection confirmed that the method, although very popular in different fields of research, is still new within soils studies in Poland. Furthermore, the method only occasionally involved arable soils. This paper briefly describes how VIS-NIRS is used in Poland and demonstrates with a few examples the main advantages of the method over classical analytical method for mineral soil analysis. As an illustration of the method potential, soil organic carbon (SOC) and clay content were predicted using partial least-square (PLS) regression at field and national scale. The models were robust at field scale and revealed a high agreement between measured and predicted values with e.g. $r^2 = 0.65$ and RMSEv = 0.11% for SOC. Prediction results at national scale are promising but less robust. VIS-NIRS is a suitable technique to estimate several soil properties at different scales and at a relatively low cost.

**Keywords:** Visible and near-infrared spectroscopy, soil spectral library, soil organic carbon, clay content

## INTRODUCTION

Visible and near-infrared spectroscopy (VIS-NIRS) is a method of choice in the agricultural sector and is actively used to determine organic compounds (García-Sanchez et al., 2017). Moreover, it is an efficient technology to investigate soils. The method has been proved effective for soil monitoring purposes (Nocita et al., 2015), soil mapping (Debaene et al., 2014a), or precision agriculture (Christy, 2008). In the last few years, the literature involving VIS-NIRS has greatly increased in number and in the diversity of the applications involved. Nevertheless, soil analysis with the method is still a challenge due to the complexity of the material matrix (Tamburini et al., 2017). In the field of soil sciences, most of the studies have focused on soil organic carbon (SOC) content prediction (Ladoni et al., 2010) because the accurate estimation of SOC is of particular interest due to its potential applications for carbon sequestration and soil quality research. Therefore, of old, there were many attempts to assess soil organic matter at low cost (e.g. Gregorich et al., 1994). Lately, many efforts are made to develop global, continental or national spectral library. A global spectral library (ICRAF, 2015) is described in details in Viscarra Rossel et al. (2016). It contains more than 23,000 spectra with several soil properties available. For Europe, the LUCAS spectral library (Stevens et al., 2013) is composed of 20,000 samples. There are also few national library e.g. Australia, Denmark, or France (Gogé et al., 2012; Knadel et al., 2012; Viscarra Rossel and Webster, 2011). The basis of VIS-NIRS is that in the NIR region, the radiation (light) is absorbed by the different covalent chemical bonds (e.g. C-H, N-H, O-H) of compounds present in the sample. The absorption intensity is related to the concentration of these compounds. Therefore, a NIR spectrum contains information about the organic composition of that sample. Physical properties (e.g. soil texture) are also related to the spectrum since the shape of the spectrum is affected by light reflection and scattering and also by clay content and mineralogy. In the VIS region (350–780 nm), most of the spectral variation between soil samples are due to organic matter and iron oxides. In the NIR region (781–2500 nm), the spectrum consists of overtones and combination bands of fundamental molecular absorptions from the mid-infrared region.

With the world's growing population, there is a need for a more productive and sustainable agriculture (Bongiovanni and Lowenberg-DeBoer, 2004). Moreover, the increase of population is also related to environmental problems such as soil pollution or global warming. Precision agricul-

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ture (PA) with the use of near-infrared sensors is one of the responses to these problems. Despite the fact that SOC has been the "core" of VIS-NIRS predictions and that the method has proved to be robust in some conditions, very few attempts have been made at homogeneous (with minimal SOC variations) soils like those from Baborówko fields. The aim of the paper is to quickly review the development of VIS-NIRS for agricultural soil analysis in Poland and through few examples illustrate how the method can be used to predict SOC and clay content at field and national scale by using the Polish Soil Spectral Library (PSSL).

## MATERIAL AND METHODS

### Web of Science query

A limited search at the Web of Science (WoS) Core Collection was undertaken (as of 01.06.2019) to see if the method is still new in the field of soil sciences and as a mean to underline the originality of this study in Poland. To simplify the analysis, the WoS query was run with two mandatory terms: (a) *near-infrared* and (b) *soil* with at least one author having a Polish address. The same query was done also with no country restriction (world) and with France to see the contribution of Poland on the field. To compare with other fields of research, the same query (within the same time laps) was undertaken with common studies in soil sciences such as *soil* + *erosion*, *soil* + *contamination* then restricted to polycyclic aromatic hydrocarbon (*soil* + *PAH*) instead of near-infrared.

### Building of the Polish soil spectral library

To build the soil spectral library, more than 2200 samples from the IUNG-PIB soil database were scanned using the Veris VIS-NIR spectrophotometer in bench top mode (Veris Technologies, USA). The samples were legacy samples (1700 samples) but also samples coming from several monitoring or investigations carried out in the IUNG-PIB experimental stations (500 samples). All samples were oven dried, ground, and sieved. For all these samples, SOC and clay content were available. Tiurin determination method (SOC) was used for all 500 Baborówko samples and most of PSSL samples (some were determined by CN analyser). Clay content was determined by laser diffractometry for Baborówko samples. Hydrometer method was used to determine clay in more than 70% of PSSL samples. Samples were placed against the face of the sapphire window in a sample holder and scanned in the 350–2220 nm range. Great care was taken to scan all samples with a similar procedure. A description of the scanning methodology can be found in (Debaene et al., 2014b). Next, the spectrum from each sample was matched with its chemical or physical properties (chemical analyses) to obtain a matrix. That matrix was later subjected to multivariate analysis.

### Calibration and sample selection

To illustrate how the method works at field scale, 200 samples from Baborówko experimental station were randomly selected from the PSSL. Spectra were pre-processed with standard normal variate (SNV) and Savitzky-Golay derivatives. Partial least square regression (PLSR) was used as a multivariate calibration method for all the following models. The PLSR determines the best relationship between chemical or physical soil properties (dependant response – Y) and spectra (predictor variable – X). The method combines the features of principal component analysis and multiple linear regression. The 200 samples were divided in two datasets: 100 calibration samples and 100 validation samples. K-means clustering algorithm was used for sample selection, according to Debaene et al., (2014a) procedure. All analyses were performed using Unscrambler X 10.3 software (Camo, Norway).

To predict SOC and clay content at national scale with PLSR, 1500 samples from the PSSL were used (topsoils 0–30 cm). Samples were selected to encompass typical Polish arable soils. Soils with high SOC or clay content were not considered (e.g. SOC > 5% and clay > 10%). A principal component analysis (PCA) on the PSSL spectra was used to detect and remove outliers. The remaining samples were sorted into ascending order of analyte content (SOC and clay) and then randomly divided into two datasets for calibration and validation (992 and 500 respectively before outlier detection).

## RESULTS

### Web of Science query

The results of the different queries are presented in Table 1. A paper from Poland means that at least one author had a Polish affiliation at the time of publication. Several times, there were cases of foreign researchers with two affiliations or Polish researchers abroad but also with two affiliations. One can see that NIR studies are very scarce in Poland and also not as popular in the world (2,824 papers) as soil contamination or erosion studies (± 35,000 papers each).

The treemap of results with Polish authors (affiliation) according to WoS is presented in Figure 1. A closer look at these results revealed that among the 34 papers, only seven papers are involved with soil studies. Ten papers are not directly related to soil science (NIR reflectance analyses of leaf, roots, lignite-humus mixtures, plant-based food and satellite imaging). Seven papers are focusing on the theoretical basis of NIR light reflectance in relation to soil surface roughness and are not involved with soil analyses or with the prediction of any soil properties (e.g. Cierniewski and Verbrugghe, 1997). There is one review (Chodak, 2008) of the possible uses of the method in environmental studies

Table 1. WoS query results.

| | Mandatory terms | | | |
|---|---|---|---|---|
| Variable | NIR + soil | Contamination + soil | PAH + soil | Erosion + soil |
| Poland | 34 | 1,261 | 178 | 375 |
| France | 275 | 1,690 | 339 | 1,709 |
| World | 2,824 | 35,348 | 4,963 | 34,343 |
| Share (world %) | 1.2 | 3.57 | 3.59 | 1.09 |
| ratio Pl/F | 0.12 | 0.75 | 0.53 | 0.22 |

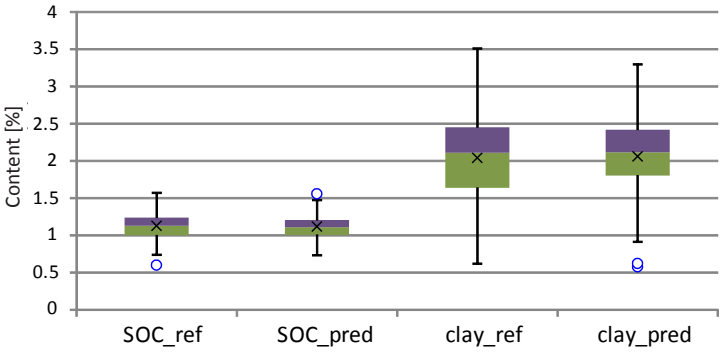
Results are in number of papers. Share is the percentage of papers with at least one Polish affiliation in %. Ratio Pl/F is the ratio of Polish to French papers.


Figure 1. Treemap of query results for „near-infrared + soil" with at least one Polish affiliation. Some papers belong to more than one categories.

and therefore also soils. The remaining articles are mostly focusing on soil properties prediction. The seminal paper related to soil properties predictions for Poland is from 2003 (Chodak et al., 2003), and like two-third of these papers, investigated forest soils. In that paper, the authors have successfully predicted many soil properties of 5 soil cores in central and northern Germany. Only four papers (Debaene et al., 2014a; Debaene et al., 2014b; Bajorski et al., 2016; Siebielec et al., 2004) studied arable soils. Many papers were authored by Polish researchers abroad e.g. (Chodak et al., 2004; Siebielec et al., 2004) due to the lack of instruments at that time in Poland.

## Prediction of SOC and clay content at field scale

Figure 2 presents the box plot of reference (measured) and predicted values for SOC and clay




The cross represents the mean; the line through the box is the median.
SOC_ref – measured SOC; SOC_pred – predicted SOC;
clay_ref – measured clay; clay_pred – predicted clay.
Blue circles are outliers.

Figure 2. Box plots of measured and predicted SOC and clay content values (Baborówko – field scale).

content for Baborówko samples (validation dataset). The results are very similar for means, medians, maximum and minimum values but the predicted clay content presents a reduced interquartile range. The results from calibration and validation for SOC and clay PLS prediction using raw spectra, SNV spectra and SG spectra are presented in Table 2. The best results were obtained with raw spectra for both properties with very low root mean square errors of prediction (0.11% for SOC and 0.33% for clay). Pretreatments of the spectra did not improve the prediction but rather lowered the robustness of the models.

The predicted vs. reference values obtained at field level are presented in Figure 3a and 3b.

Table 2. Calibration and validation results for SOC and clay content prediction (Baborówko – field scale).

| | $r^2$ | RMSE [%] | $r^2$ | RMSE [%] |
|---|---|---|---|---|
| | SOC | | Clay | |
| Calibration (n = 100) | | | | |
| Raw | 0.73 | 0.14 | 0.87 | 0.23 |
| SNV | 0.78 | 0.14 | 0.78 | 0.30 |
| SG | 0.77 | 0.13 | 0.88 | 0.22 |
| Validation (n = 100) | | | | |
| Raw | **0.65** | **0.11** | **0.77** | **0.33** |
| SNV | 0.33 | 0.63 | 0.65 | 0.45 |
| SG | 0.61 | 0.15 | 0.47 | 0.51 |

Raw – raw spectra, SNV – standard normal variate, SG – Savitzky-Golay derivative

**PSSL and SOC and clay prediction (National scale)**

Figure 4 presents the Hotelling $T^2$ ellipse with 95% confidence interval on the score plot from the PCA analysis of the PSSL spectra. The Hotelling $T^2$ is a linear function of the leverage that can be compared to a critical limit according to an F-test. This statistic is useful for the detection of outliers at the modelling or prediction stage. Two hundreds samples were considered as outliers (outside of the ellipse or with SOC > 5% and clay > 10%) and therefore removed from the modelling. These are samples not representative of Polish arable soils. After outliers detection, 892 samples were used for calibration and 400 samples for validation. The two first components (PC-1 and PC-2) concentrate 99% of data variation. Samples outside the boundaries of the Hotelling ellipse were considered as spectroscopic outliers. Samples are clustering according to spectral similarities due to e.g. SOC or clay content.

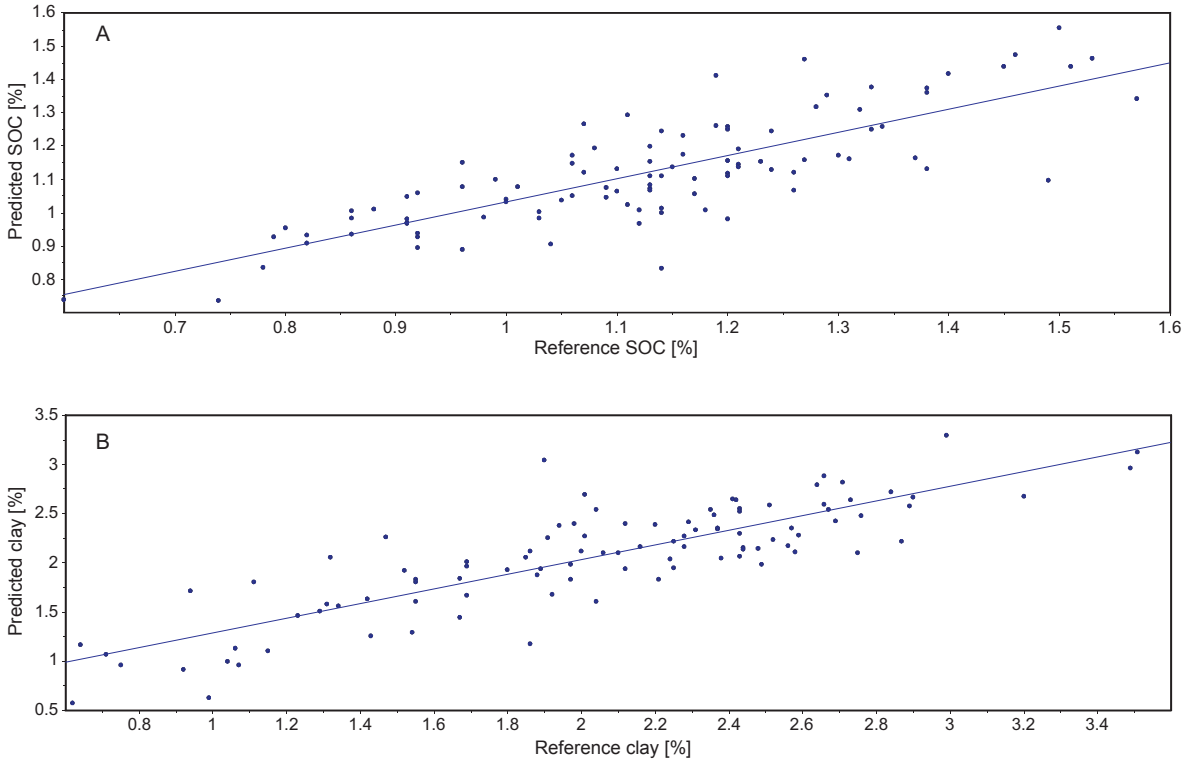



Figure 3. Measured vs. predicted SOC (A) and clay content (B) for Baborówko samples. Validation models with raw spectra.

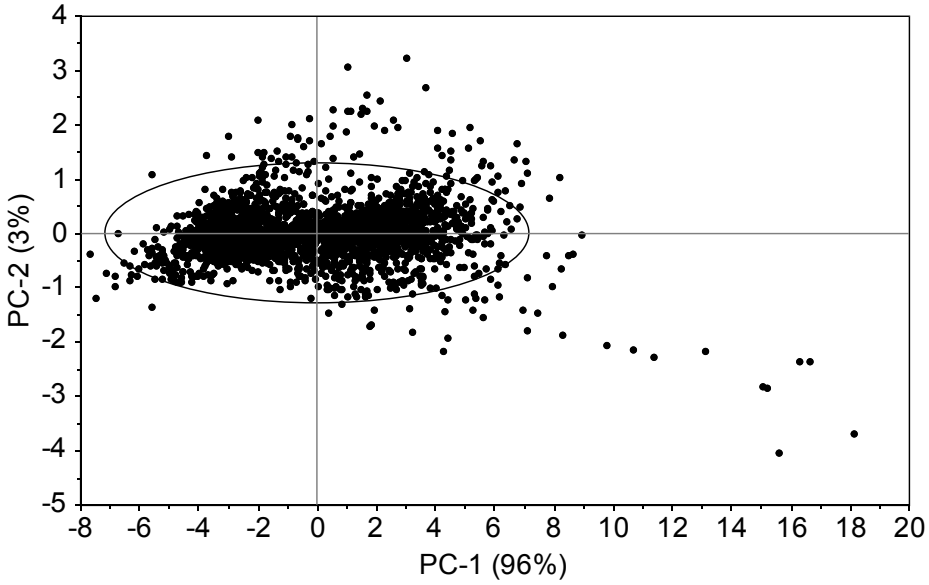



Figure 4. Spectra PCA-scores with Hotelling $T^2$ ellipse (95% confidence interval).
PC – principal component

The best models were obtained using SNV pre-processing. Modelling results for SOC were the following: $r^2$ = 0.69 and RMSE = 0.60% for calibration and $r^2$ = 0.66 and RMSE = 0.61% for validation. Prediction results for clay content were similar: $r^2$ = 0.73 and RMSE = 0.91% for calibration and $r^2$ = 0.71 and RMSE = 0.88% for validation.

## DISCUSSION

The WoS analysis has revealed the relative novelty of the method in the field of soil sciences, especially in Poland were only 34 papers were published until now. Many papers were authored by Polish researchers abroad or foreign researchers in Poland but with two affiliations. Moreover, researches involving VIS-NIRS represent less than 3% of e.g. the number of studies concentrating on soil contamination or 19% of soil PAH's studies in Poland. The results also highlighted a common misunderstanding concerning the method: the difference between proximal and remote sensing (see Anastasiou et al., 2018). More than half of the 34 papers involved remote sensing studies and not VIS-NIRS studies. The other half of the papers are dealing with forest soils and only four papers are discussing arable soils in relation with VIS-NIRS which support the utility of the present work and explain the growing interest for the method in many Polish Universities and Institutes. This also justifies further investigations are needed since precision agriculture is mostly focusing on arable mineral soils.

Prediction results at the field scale (Baborówko study) have confirmed the robustness of the method for SOC and clay prediction. One hundred samples were used for calibration to predict 100 independent (new) samples. This means that after building the calibration model, the analytical costs for the determination of SOC and clay were reduced by 50%. Moreover, once a model is robust and can be used in a more routine approach, all new samples only need to be scanned and incorporated in the model for prediction. This further decrease overall cost analysis. It was determined by Nduwamungu et al., (2009) and Debaene et al., (2014a) that for Canada, France, and Poland the costs are reduced by 63%, 94%, and 80% respectively in comparison to certified laboratory using classical methods. After an initial relatively high cost for calibration since classical laboratory analyses are needed, the more samples predicted with a model, the lower the costs will be. In the case were a model is robust enough to be used in routine analysis like it is the case in the cereal industry (Delwiche, 2004), the costs are drastically lowered. Unfortunately, soil is a complex material and such a model is not relevant at larger scale and probably will not be achieved soon or ever (Stevens et al., 2013). Nevertheless, local models (field or farm level) are applicable and proved robust enough for precise determination of several soil properties (Stenberg et al., 2010). These models can be used for mapping and precision agriculture. Comparable prediction results to Baborówko field models were obtained by Dunn et al., (2002) for Australian topsoils of very similar composition and by Debaene et al., (2014a) on 400 samples from a georeferenced grid sampling investigation in Baborówko farm. Such very small prediction errors (RMSE) of 0.11% are seldom reported in the literature and that precision is simi-

lar to classical methods of SOC determination (Jankauskas et al., 2006). However, it is to be noticed that the small RMSE here is also related to the fact that the range of SOC values in both calibration and validation dataset is narrow. Despite the fact that spectra pre-processing is an important chemometric tool (Rinnan et al., 2009), there were no improvement when pre-processing the spectra of Baborówko samples. This was reported elsewhere (Freschet et al., 2011; Zornoza et al., 2008) for SOC or total C and N content. In the present case, this is probably due to the field's relatively homogeneous texture that preserved samples from excessive light scattering.

The costs of developing a soil spectral library are elevated. This is the reason why the present PSSL was built using legacy samples from the IUNG-PIB soil database and samples from different IUNG-PIB experimental stations. This is probably why most of spectral library are developed that way (Viscarra Rossel and Webster, 2011). Using legacy soil databases is associated with errors related to the fact that several analytical technics can be used for soil analysis e.g. SOC can be analysed by Tiurin method or by Walkey--Black method (Soriano-Disla et al., 2014). This was the case here where samples from the PSSL were analysed for SOC and clay with different methods. This can explain why the RMSE errors and robustness of the prediction models are lower than Baborówko models where only one method of determination was used. Probably, using only the samples analysed with one method for SOC or clay content could greatly improve the predictions but would be less realistic. Besides, the larger the scale of investigation, the higher prediction errors are since the range of soil properties values is, and the range of soil types involved is wider (SOC content = 2.15% and clay content = 3.11% in this dataset). Therefore, a large spectral database increases the chances of having non-representative validation samples. That problem was relatively bypassed by choosing only typical samples for Polish arable soils and deleting samples with extreme SOC and clay values. Incorporating these samples in the model would probably have increased RMSE greatly. Nevertheless, when compared with other large-scale studies (e.g. Brown et al., 2005; Gogé et al., 2012) the obtained errors are smaller. The PSSL is a new national spectral library that is expanding the range/choice of the available national libraries e.g. Denmark, France, or Australia (Gogé et al., 2012; Knadel et al., 2012; Viscarra Rossel and Webster, 2011).

The building of the Polish Soil Spectral Library is an ongoing project and new samples are regularly incorporated and calibration models updated to obtain more robust VIS-NIRS models at national scale. The PSSL could be used as a tool for e.g. monitoring carbon stock, an important factor of climate change. Other soil properties are also investigated and prediction models developed.

## CONCLUSIONS

The present paper illustrated the use of a large-scale spectral library (PSSL) to predict two of the main soil properties (SOC and clay content) in arable mineral soils at field and national scale. The method is useful for mapping and precision agriculture as well as soil monitoring. The main conclusions are:

1. The method is still relatively new in Poland for the determination of soil properties as was demonstrated by the Web od Science query when compared to France or the entire world. More investigations are needed in that field of research with more soil types and at different scales.
2. The robustness of the method is better at field or farm scale than at national scale and with precision comparable to classical analytical techniques. However, the main advantages over classical methods is the rapidity, the low cost of analysis (50% to 90% cheaper) and the fact that no environmentally harmful chemicals are needed.
3. SOC and clay content can be predicted at different scales and with low errors at field scale.
4. The building of a spectral library is a continuous process and including new samples with different range of values is a requirement to predict new soil types and obtain more robust prediction models.

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