NEAR-INFRARED REFLECTANCE SPECTROSCOPY FOR ESTIMATING SOIL CHARACTERISTICS USEFUL IN THE DIAGNOSIS OF SOIL FERTILITY

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Objectives

The objective of our work is to contribute to the implementation of a general procedure for soil fertility diagnosis (i) for routine work in the soil analysis laboratories of the Walloon REQUASUD network (Southern Belgium), (ii) without extra cost for laboratories and/or farmers, and (iii) which meets the current agronomic and environmental requirements. This study focused on the ability of near-infrared reflectance spectroscopy (NIRS) to predict soil total organic carbon (TOC), total nitrogen (TN), clay content, and cation-exchange capacity (CEC). This study deals with the considerations related to the adjustment of a methodology for the implementation of a spectral library and calibration of predictive models.

Materials and methods

The methodology developed to build the most accurate models for predicting those soil properties includes the following steps:

1. Evaluation of the population diversity for the four studied soil characteristics in Wallonia (Fig. 1)
2. Set-up of a representative sample set from this population
3. Analysis of the samples following standard procedures
4. Division of sample set between calibration, tuning and validation subsets (Fig. 2)
5. Elaboration of a procedure for soil sample preparation prior to scanning (Fig. 3)
6. Scan in replicate all the samples following this procedure
7. Elaboration of a predictive model for each soil characteristic based on the local PLS regression in comparison to the classic PLS regression (Fig. 4)
8. Evaluation of the repeatability and reproducibility of the method

Fig. 3: The procedure for soil sample preparation

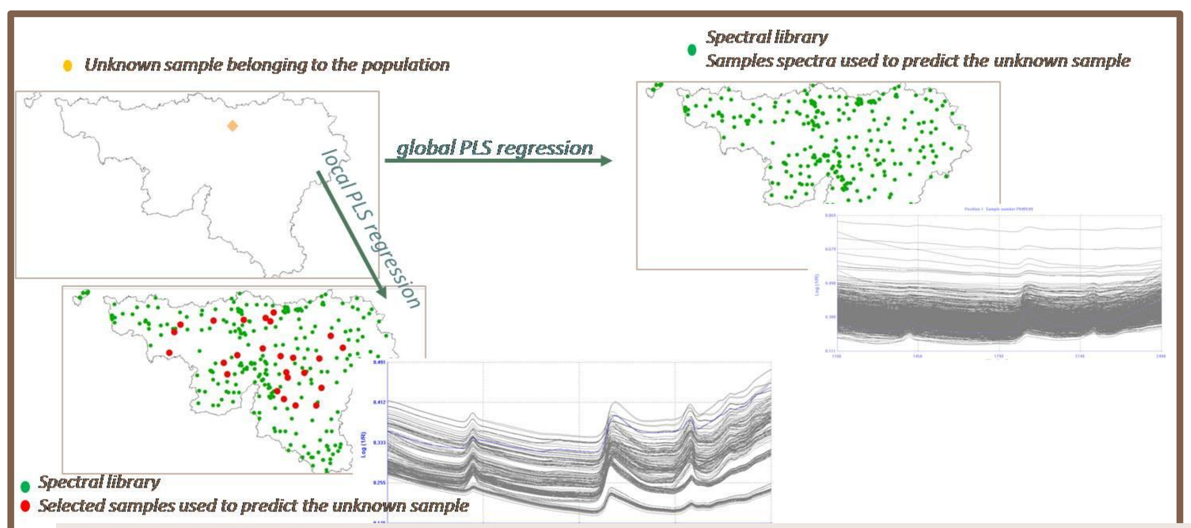

Fig. 4. Comparison between the global and local PLS regression

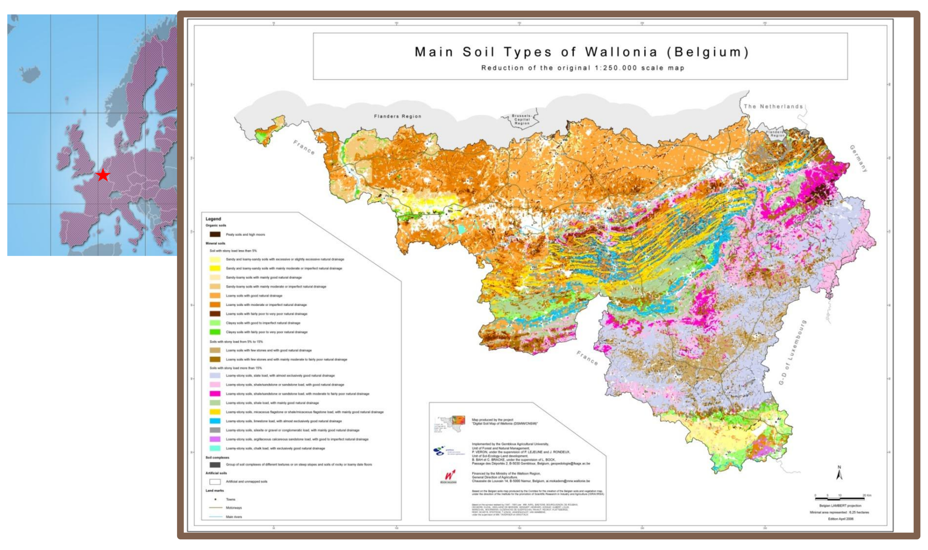

Fig. 1: Main Soil Types of Wallonia (Belgium). Reduction of the original 1:250,000 map

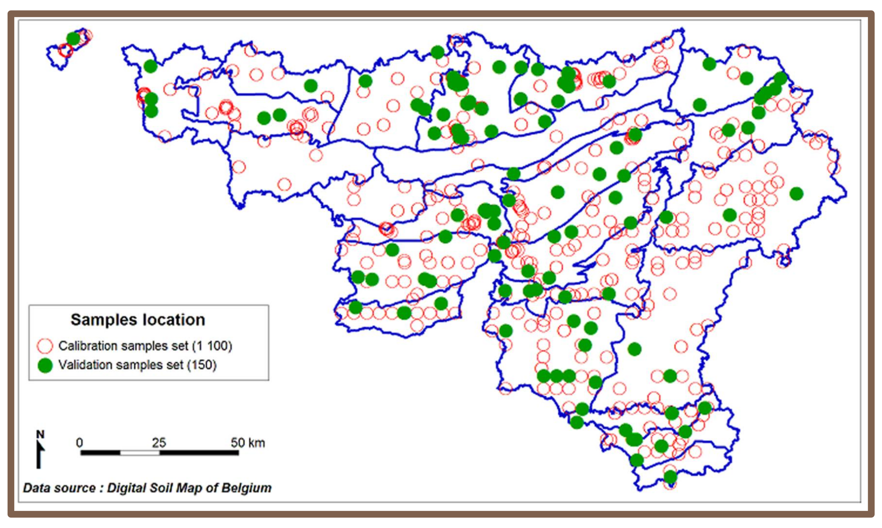

Fig. 2: Location of the calibration and validation sample sets in the various landscape units of Walloon Region

The PLS local regression matches the sample to be predicted with a small homogeneous group of samples selected from the calibration set. Each unknown sample is compared to the calibration set and the closest samples are selected from the spectra database. Then, based on selected samples, a new equation is built to predict the sample. The similarity index used to choose the small homogeneous group of samples is simply a correlation coefficient between spectra.

Results and discussion

The following graphics (Fig. 5) collate the results obtained for the best global PLS model (by comparing 15 spectra pre-treatment) with the reference methods. It can be noticed that the cloud of points obtained for TOC and clay content present a wider scattering with increasing values. On the contrary, the clouds of points obtained for TN content and CEC are independent of the data range.

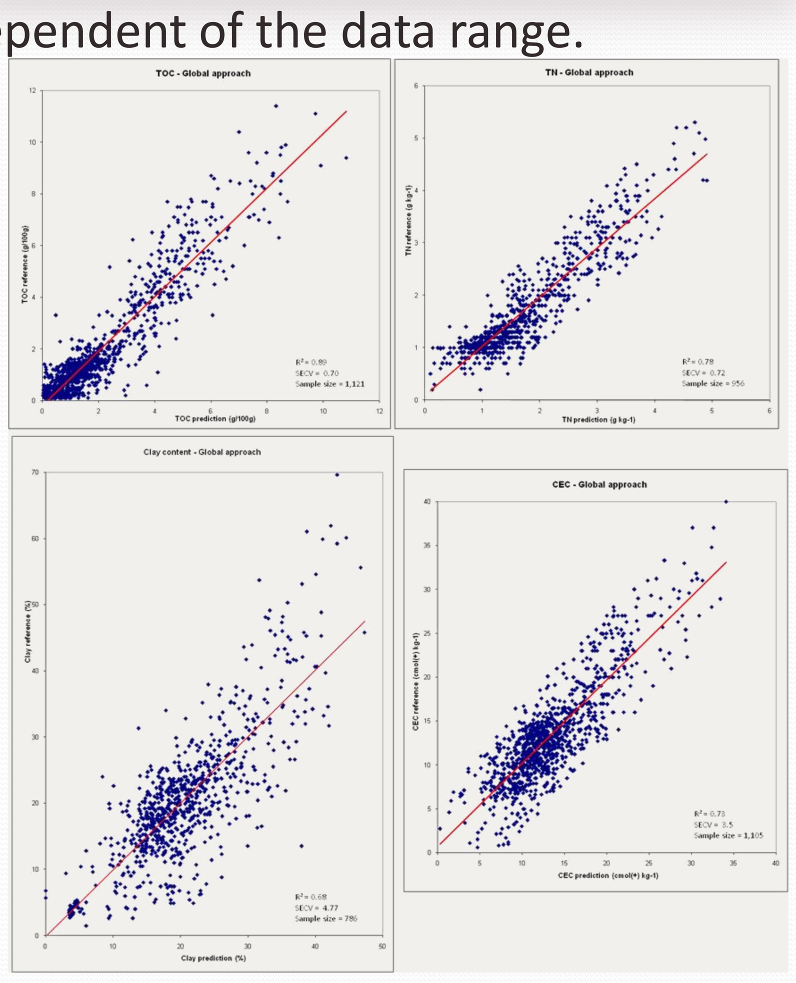

Fig. 5: Relationship between the reference results and the predicted ones for the most accurate pre-treatment in the calibration approach (first minimum of SECV)

Comparing the SEP (standard error of prediction) or CVp (coefficient variation for the prediction) obtained with PLS global model to that with PLS local regression without any fixed similarity index (no r²-value), showed that prediction accuracy was improved for each soil characteristic, except for the TOC content. The CVp for global and local models are 30% / 39%, 65% / 36%, 27% / 24% and 34% / 25% for TOC, TN, clay content, and CEC, respectively. By increasing the similarity index value until 0.99, the accuracy of the models was improved to obtain a CVp of 10 % on average but the number of predicted samples decreased significantly; only one third of the samples, essentially crop soil samples, being well predicted (Fig. 6).

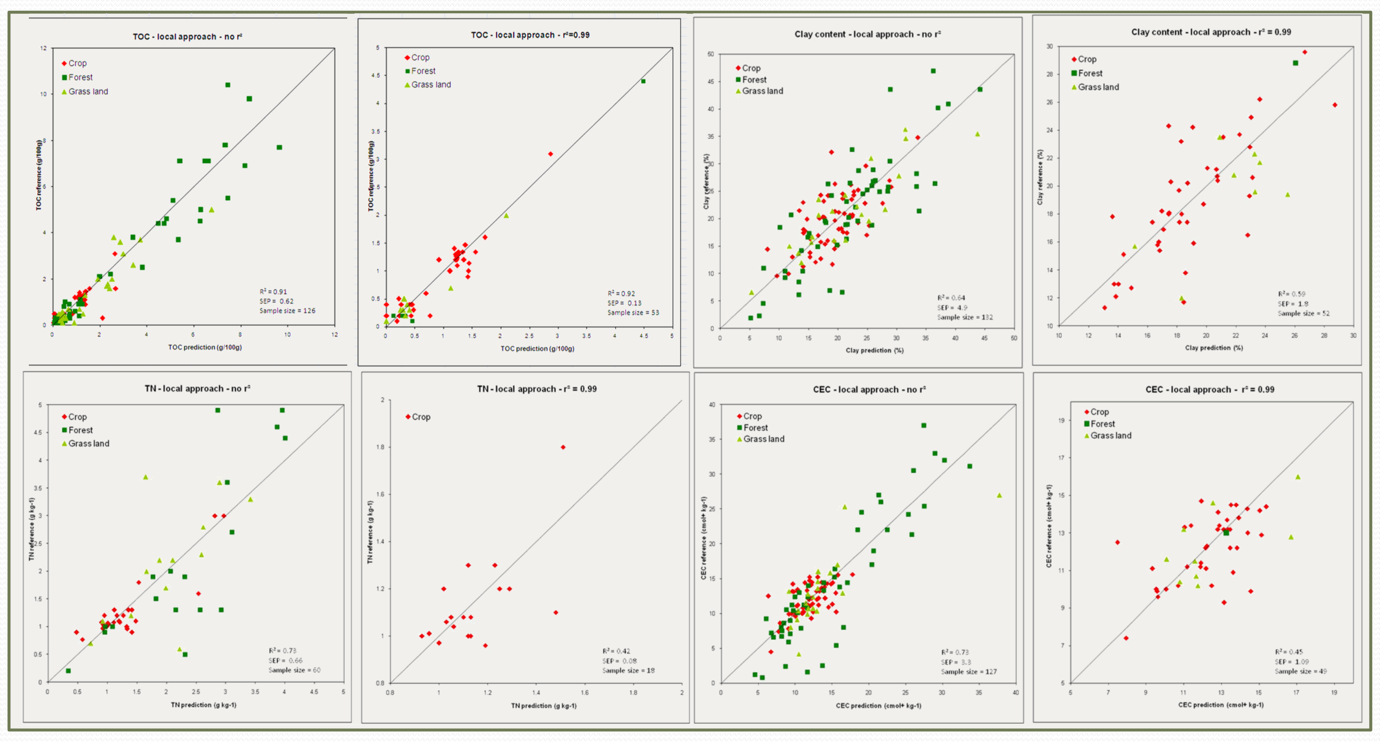

Fig. 6: Results of the PLS "local" regression models for the validation sample set

The study of the repeatability and reproducibility of the NIRS technique indicates that NIRS analysis is as reliable as the analytical methods for determination of TOC, TN, clay content and CEC (Table 1). The weight of the repeatability and reproducibility standard error in the SEP were also evaluated. Even if this equation is an approximation, the results indicate that the parts of the reproducibility error due to NIRS and to analytical methods are negligible in comparison to the lack of fit for the four studied soil properties (Table 2).

Table 1: Results of the repeatability and intra-laboratory reproducibility studies for TOC, T N, clay content, and CEC

	Repeatability				Reproductibility			
	sr	sr%	r	r%	sR	sR%	R	R%
TOC content (g $100g^{-1}$)	0.001	1.62	0.11	4.48	0.008	3.82	0.25	10.59
TN content (g kg^{-1})	0.002	1.55	0.12	4.30	0.005	2.63	0.20	7.29
Clay content (%)	0.83	3.50	2.30	9.71	1.82	7.67	5.04	21.27
CEC (cmol(+) kg^{-1})	0.19	2.49	1.22	6.91	0.81	5.10	2.49	14.14

sr = standard error of repeatability – sR = standard error of reproducibility
r = repeatability – R = reproducibility

Table 2: Weight of the standard error of reproducibility (sR)in the SEP in comparison to the lack of fit (slf) and the reproducibility analytical error (sRa).

	SEP	sR	sRa	slf
TOC content (g $100g^{-1}$)	0.62	0.008	0.03	0.61
TN content (g kg^{-1})	0.66	0.005	0.05	0.65
Clay content (%)	4.9	1.82	2.0	4.3
CEC (cmol(+) kg^{-1})	3.3	0.81	1.3	3.0

SEP = standard error of prediction
sR = standard error of reproducibility
sRa = standard error of reproducibility for the Soil Science Laboratory of Gembloux
Slf = lack of fit

Conclusion

The main conclusions of our study are:

(i) The variations of predictive accuracy of the 15 spectra pre-treatments were rather small. CV_{CV} (coefficient variation for the cross validation) values were ranging between 35 and 50% for TOC and TN, between 20 and 30% for clay content and CEC. No unique solution could be found to minimize simultaneously the four soil properties, nor calibration and validation subsets.

(ii) The PLS local models, using a similarity index of 0.99, give the most accurate results for the four soil properties, in comparison to the global PLS regression. In Walloon Region, it is thus recommended for routine work to apply the PLS local model with this similarity index.

(iii) The repeatability and reproducibility of the NIRS technique are similar to those obtained following chemical analysis.

Results confirm that NIR spectroscopy can be used as a rapid analytical technique to simultaneously estimate soil TOC, TN, clay content, and CEC with acceptable accuracy, as shown by other authors in different situations. As clay content and CEC considered for the assessment of the nutrient level are usually rough estimates, the use of NIRS estimates should improve the fertility diagnosis for sandy and clayey soils, as well as for many loamy-stony soils.

At present, only the soil crop samples are well predicted for the four studied soil characteristics. The lack of samples covering the diversity of the grasslands and forests soils could explain that few of them are well-predicted.

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