AGRICULTURAL SCIENCE AND TECHNOLOGY, VOL. 1, № 2, pp 1-6, 2009

Determination of soil organic carbon using near-infrared spectroscopy

M.Todorova, [1*] S. Atanassova [1], R. Ilieva [2]

[1]Department of Plant Science, Faculty of Agriculture, Trakia University, 6000 Stara Zagora, Bulgaria
[2]Institute of Soil Science "N. Poushkarov",7, Shousse Bankya Str., 1080 Sofia, Bulgaria

(Manuscript received 9 June 2009; accepted for publication 14 July 2009)

Abstract. *The usefulness and limitations of near infrared reflectance spectroscopy (NIRS) for the analysis of soil are still not sufficiently explored. The objective of this study is to evaluate the ability of NIRS to determine the organic carbon in several different soil types. A total of 138 soil samples of Vertisols, Chernozems, Fluvisols and Luvisols, were taken from 0-60 cm layer. The organic carbon content was determined by the Tyurin method. Soil spectra were collected using InfraAlayzer 450 spectrophotometer within the range of 1445-2348 nm. Calibration equations for determination of soil organic C content were derived by MLR using two/third of the samples as calibration set and tested with the rest of the samples as independent validation set. In order to compare spectral characteristics of the samples from different soil units principal component analysis was used. Soil samples were classified in a space of PC according to their NIR spectra into several groups. The samples of Vertisols and Chernozems formed clearly separated groups. Fluvisols and Luvisols samples were spectrum similar and formed one group. For the global calibration, containing the samples of all soil units, the standard error of calibration (SEC) and of prediction (SEP) were 0.32 and 0.37%. The ratio of the standard variation of the reference data to the SEC or SEP (RPD), indicating the performance of calibration, was 2.13 and 1.92, respectively. Dividing the samples into groups according to their spectral similarity can improve the prediction accuracy. For example, for a group of spectrum similar samples of Fluvisols and Luvisols SEC and SEP was 0.18, RPD for validation was 3.00. This study shows that NIRS can be used as a fast and routine method for prediction of soil organic C.*

Keywords: non-destructive method, soil organic matter

Introduction

Near-infrared spectroscopy (NIRS) is an analytical technique known for its rapidity, simplicity and cost-effectiveness. NIRS utilizes electromagnetic spectra in the region 700-2500 nm. Near-infrared reflectance spectroscopy is based on the absorption of C-H, N-H and O-H groups found mainly in organic constituents. These absorptions are the overtones and combination of fundamental vibration bands in the mid-infrared spectral region. The extraction of useful information contained in optical spectra must be done by using chemometric technique such as multiple linear regression, principal component regression and partial least squares regression.

This technique has been widely used for several decades for analysis of different agricultural products such as grains, forages, milk, food etc. (Williams and Norris, 2001; Gonzalez-Martın et al, 2008). Recently, there is a growing interest in using NIRS for soil analysis.(Chang C, 2001; Confalonieri M et al, 2001; Bogrekci I and Lee S, 2004; Siebielec et al, 2004; Yong et al, 2005;Cozzolino and Moron, 2006; Mouazen et al, 2006; Zornoza et al. 2008; Terhoven-Urselmans et al, 2008)

The objective of this study was to evaluate the ability of NIRS for quantitative determination of organic carbon in soil samples from different soil units.

Material and Methods

Soil samples

A total of 177 samples from the 0-20 and 40-60 cm layer were collected from different regions in Bulgaria during April - October, 2007. Soil types were Calcic Chernozems and Eutric Chernozems from North Bulgaria, Calcic Vertisols and Eutric Vertisols, Chromic Luvisols and Calcic Fluvisols (FAO, 1998) from South Bulgaria, which are main soil types in Bulgaria. The samples were analysed for organic carbon content by Tyurin method.

Spectral analysis

NIR spectra of all samples were obtained by InfraAlyzer 450 filter-type spectrophotometer within the range of 1445-2348 nm. Two or three measurements were carried out for each soil sample using independent sampler cell fillings and then averaged to give one spectrum per sample. Six calibration equations were composed for quantitative determination of organic carbon in different sets of soil units. Calibration equations were derived by multiple linear regression. Two-thirds of the samples of every soil set was used as a calibration set, and the remaining samples as an independent test set. The number of soil samples of Chernozems and Vertisols were relatively small; respectively 40 and 42, and only calibration equations were obtained.

* e-mail: todorova72@yahoo.com

Results and discussion

The spectra of soil samples from 0-20 cm and 40-60 cm depth, respectively of Chernozems, Fluvisols and Vertisols are shown in Figure 1. All soil spectra have three large absorption peaks in the near-infrared region around 1450, 1940 and 2200 nm. These absorption features are typical for soils. The NIR absorption at 1450 nm are connected with absorption of OH first overtone, related to water, 1940 nm – combination of OH stretch plus OH bending vibrations, at 2200 nm and 2300 nm are due to the combination Al–OH bend plus O–H stretch. We can also see a distinct difference in soil spectra between the soil from different soil units. Vertisols are showing more intense absorption peak at 1940 nm, than Chernozems and Fluvisols, due to the high montmorillonite content. These lattice clay minerals are characterized by varying amounts of isomorphus substitution in both the tetrahedral and octahedral sheets; hence the spectra of Vertisols are influenced by water molecules, which are absorbed between the sheets of the

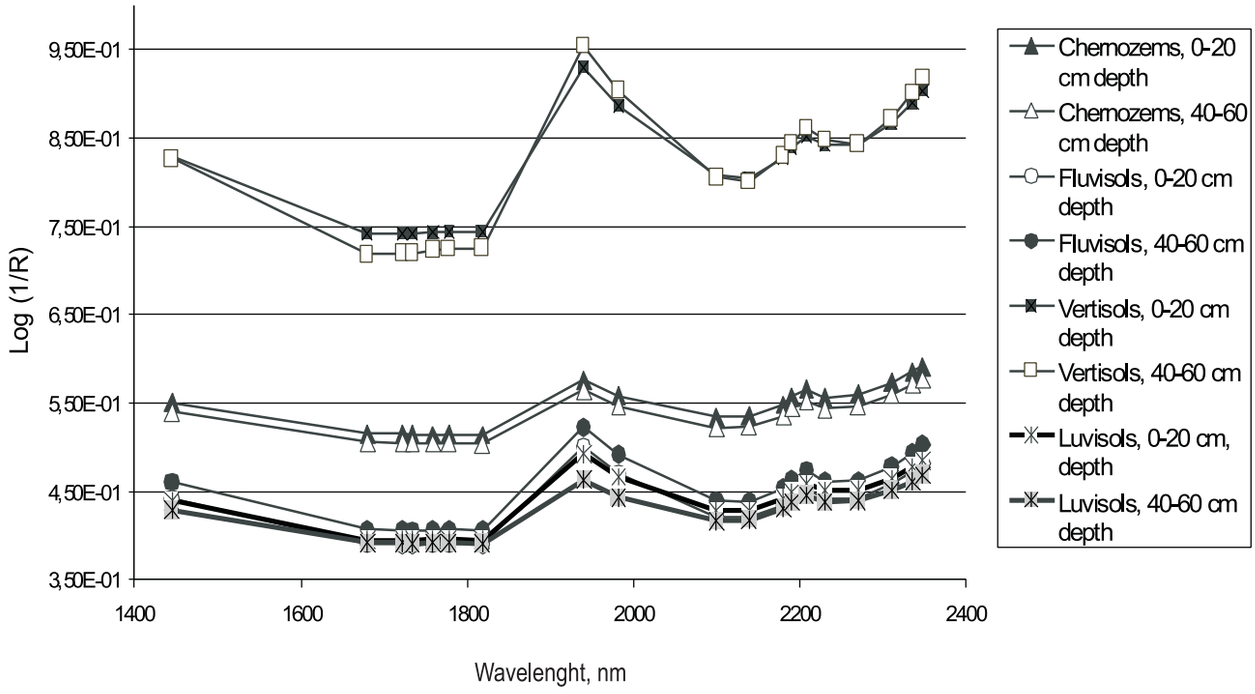

Figure 1. Spectra of soil samples from different soil units.

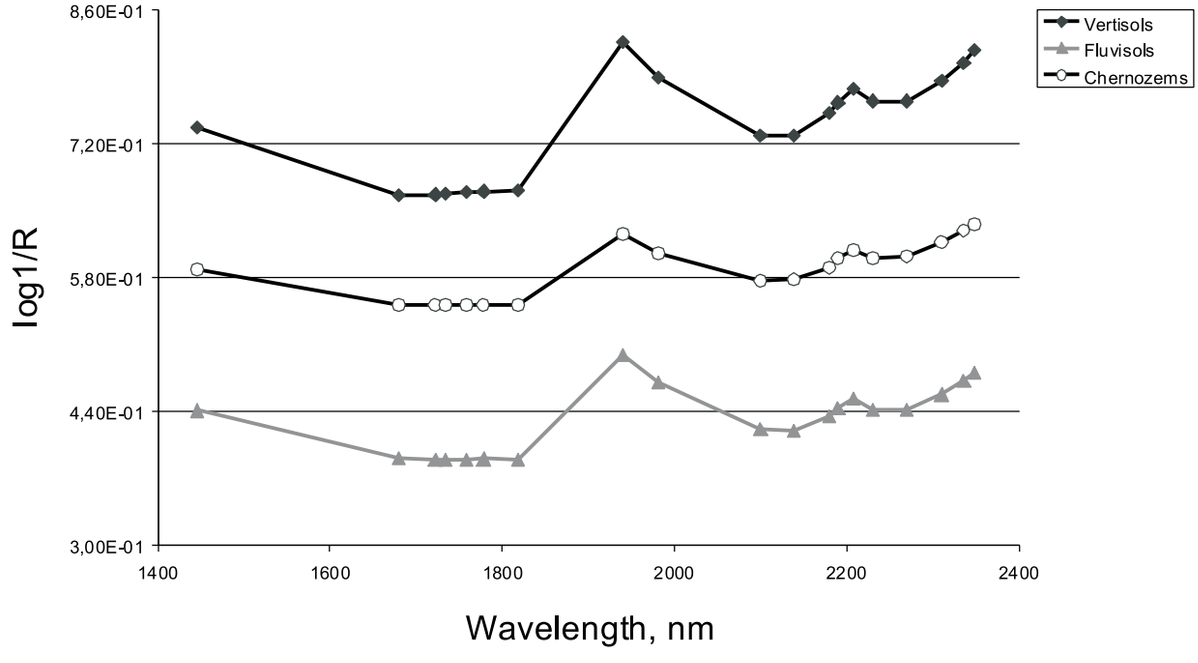

Figure. 2. Spectra of soil samples with 1,2 % organic carbon content.

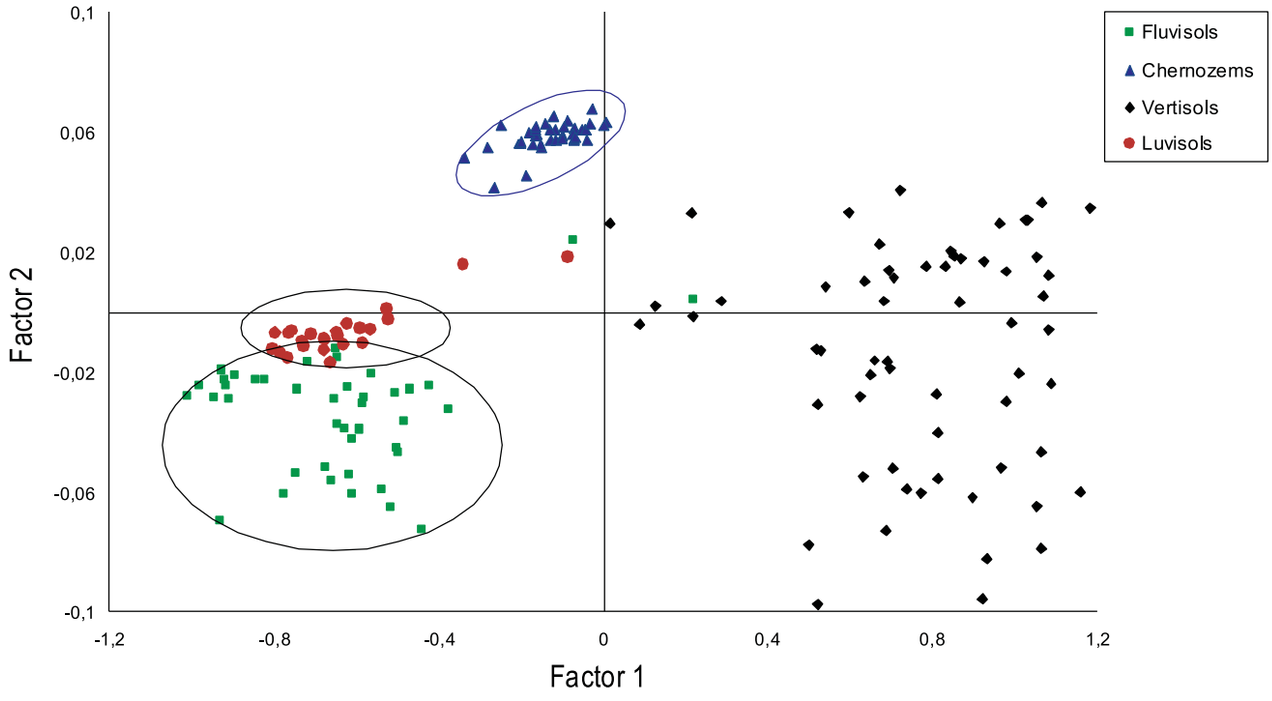

Figure 3. Score plot of the samples on the first two principal components.

Table 1. Range, mean and standard deviation (SD) of organic carbon content, % in examined samples.

	Calibration set					Test set			
Set of Soil units	n	min	max	mean	SD	min	max	mean	SD
Chernozems	40	0,52	2,70	1,42	0,53				
Vertisols	42	0,42	4.50	1,58	0,90				
Vertisols, Chernozems	82	0,42	4,50	1,57	0,79	0,42	4.50	1,62	0,71
Fluvisols, Luvisols	95	0.63	3.07	1.68	0.49	0.63	2.67	1.64	0.53
Vertisols, Luvisols, Fluvisols	137	0.41	4.52	1.56	0.72	0.58	4.52	1.6	0.74
Vertisols, Luvisols, Fluvisols, Chernozems	177	0.41	4.52	1.40	0.68	0.41	4.52	1.43	0.71

Table 2. Statistical data of the calibration equations and validation statistics for NIRS prediction of organic carbon content, % in examined samples.

	Calibration set				Test set			
Set of Soil units	n	SEC	R	RPD	n	SEP	r	RPD
Chernozems	40	0,25	0,88	2.12				
Vertisols	42	0,38	0,86	2,40				
Vertisols, Chernozems	54	0,38	0,86	2,08	28	0,42	0,84	1,80
Fluvisols Luvisols	64	0 18	0 93	2 72	31	0 18	0 95	3 00
Vertisols, Luvisols, Fluvisols	91	0.27	0.93	2.67	46	0.35	0.90	2.1
Vertisols, Luvisols, Fluvisols, Chernozems	118	0.32	0.89	2.13	59	0.37	0.86	1.92

monmorillonite structure (Viscarra - Rossel et al, 2006).

Spectra of soil samples with equal organic carbon content, but from different soil types are presented in Figure 2. The obtained soil spectra depended much more on the mineral composition of the different soil than on the organic carbon content. The spectral feature of soil organic carbon was not directly visible in the spectra. That requires sophisticated statistical techniques for quantitative spectral analysis of soil to discern the response of soil attributes from spectral characteristics. Principal component analyses were performed of all soil spectra to investigate sample distribution. carbon content in contrast to Chernozems, Fluvisols and Luvisols. In all sets of soil units the correlation coefficients between the measured and predicted values on the basis of their spectral data for organic carbon content were greater than 0.84 for both calibration and test sets (Table 2). The standard error of calibration (SEC) varied from 0.18 to 0.38%, and standard error of prediction (SEP) varied from 0.18 to 0.42, depending on soil units and the combination of soil units in sample sets. For the global calibration containing samples of all soil units, SEC and SEP were 0.32 and 0.37% and RPD was 2.13 and 1.92, respectively. The parameter RPD is the ratio between SD and SEC or SEP and indicated the performance of the calibration equations. According to Viscarra - Rossel (2007) RPD values were classified following levels of prediction accuracy: RPD between 1.5 and 2.0 indicates poor Factors 1 and 2 (Figure 3) explained 99.91% of the total variance in spectral data and separated soils into several groups, according to the unit. The Chernozems formed a fairly tight group, distant from the others. Soil samples from Fluvisols and Luvisols formed two groups at a short distance. Therefore samples of Fluvisols and Luvisols could be grouped together in a successful total calibration set for determine the soil parameter. The Vertisols samples were located in one group, different from all other soil types.

Descriptive statistics of soil OC content for each set of data are shown in Table 1. Vertisols exhibit a wide range of soil organic predictions, RPD between 2.0 and 2.5 indicates good prediction and RPD>2,5 indicates very good /excellent model/ prediction. According to those criteria, calibration equations for prediction of organic carbon showed good or very good prediction ability.

Dividing the samples into groups according to their spectral similarity improved prediction accuracy. That's why the best accuracy in determining organic carbon was obtained for the set of Fluvisols and Luvisols - SEC and SEP was 0.18 %, RPD for calibration and validation was higher than 2.5 – 2.72 and 3.00, respectively.

Figures 4 and 5 graphically illustrate the relationship between determined and NIR spectroscopy predicted values of organic content determination in two different data set.

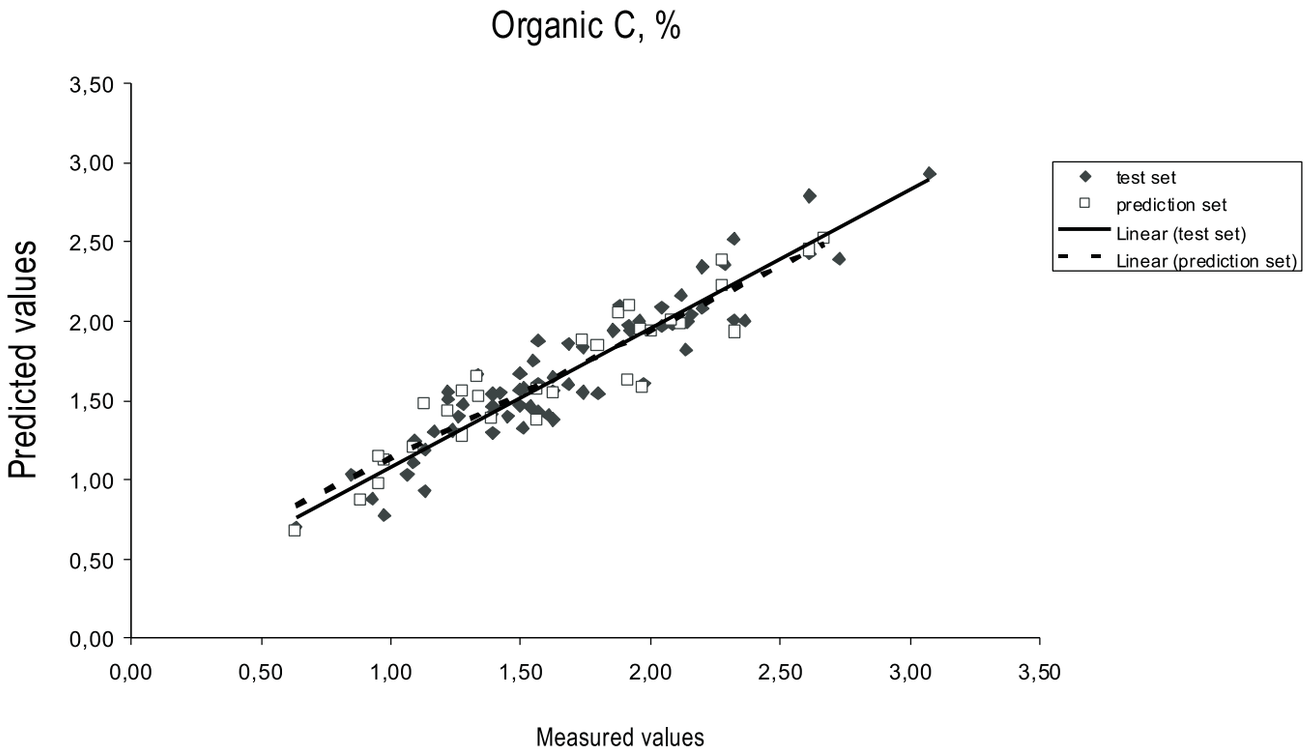

Figure 4. Relation between actual and NIRS predicted values of soil organic content in Fluvi sols and Luvisols.

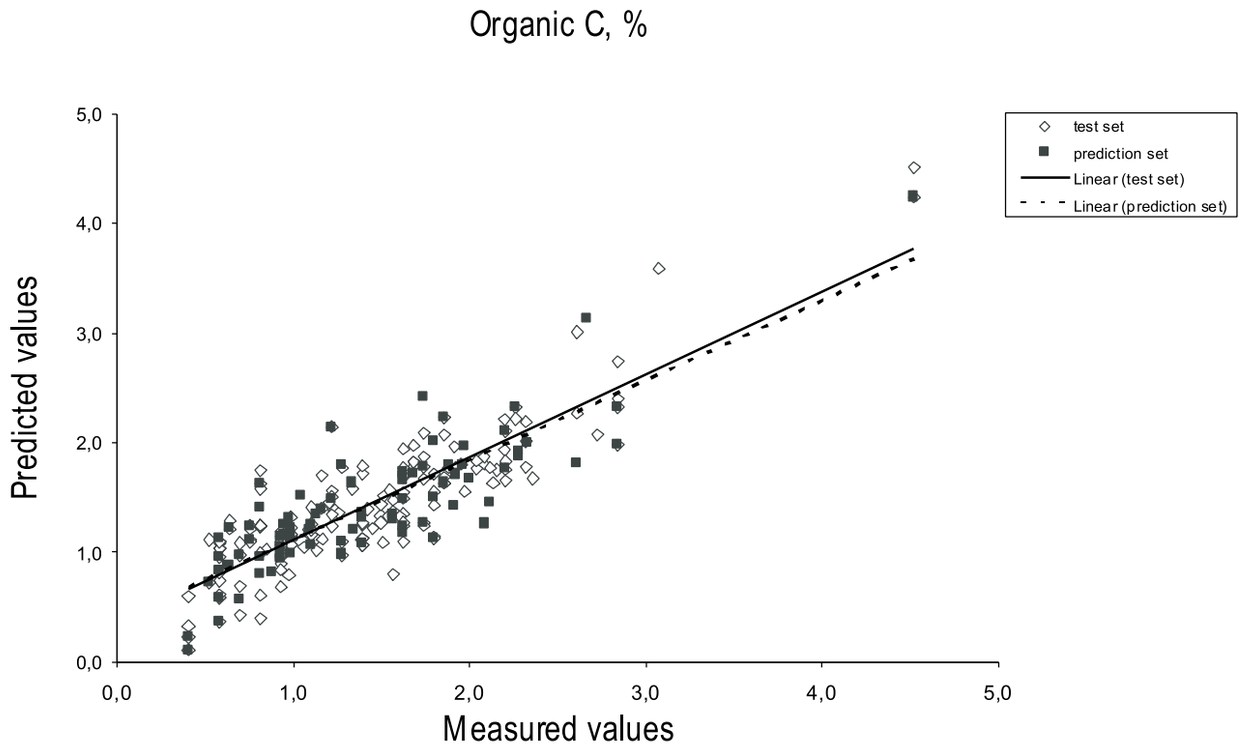

Figure 5. Relation between actual and NIRS predicted values of soil organic content in Chernozems, Vertisols, Fluvisols and Luvisols.

Conclusion

According this investigation results, NIR spectroscopy is a technique that can be considered with good potential to assess soil organic carbon in different soil units. Dividing the samples into groups according to their spectral similarity improved prediction accuracy of soil organic carbon determination.

Furthermore, the technique is rapid, making it possible to analyse a large number of samples in a practical and timely manner. These properties make spectroscopic analyses combined with chemometric methods very attractive for environmental monitoring, modelling and precision agriculture.

Acknowledgements

The authors gratefully acknowledge the financial support of the National Science Fund USS- 401/2006.

References

Bogrekci I and Lee S, 2004. Determining phosphorus concentration using spectral reflectance of grass and soil samples in the Lake Okeechobee basins in UV, VIS, and NIR regions. Proceedings of the 7th International Conference on Precision Agriculture and Other Precision Resources Management, Hyatt Regency, Minneapolis, MN, USA, 25-28 July, 2004, 1552-1560.

Chang C, Laird D, Maurice A, Maubach J, Charles R and Hurburg Jr, 2001. Near-infrared reflectance spectroscopy - Principal components regression analyses of soil properties. Soil Science Society American Journal, 65, 480-490.

Chang C and Laird D, 2002. Near-infrared reflectance spectroscopic analylisis of soil C and N. Soil Science, 167, 110-116.

Confalonieri M, Fornasier F, Ursino A, Boccardi F, Pintus B and Odoardi M, 2001. The potential of near infrared reflectance spectroscopy as a tool for the chemical characterization of agricultural soils. Journal Near Infrared Spectroscopy, 9, 123-131.

Cozzolino D and Moron A, 2006. Potential of near-infrared reflectance spectroscopy and chemometrics to predict soil organic carbon fractions. Soil and Tillage Research, 85, 1-2, 78-85.

González-Martín I, González-Pérez C, Hernández-Hierro J and González-Cabrera J, 2008. Use of NIRS technology with a remote reflectance fibre-optic probe for predicting major components in cheese. Talanta 75, 351–355.

Mouazen A, Baerdemaeker J and Ramon H, 2006. Effect of wavelength range on the measurement accuracy of some selected soil constituents using visual near-infrared spectroscopy. Journal Near Infrared Spectroscopy,14, 189-199.

Siebielec G. McCarty T, Stuczynski and Reeves J, 2004. Near- and mid-infrared diffuse reflectance spectroscopy for measuring soil metal content. Journal of Environmental Quality, 33, 2056-2069.

Yong He, Song H, Pereira A and Gomez A, 2005. Measurement and analysis of soil nitrogen and organic matter content using near-infrared spectroscopy techniques. Journal of Zhejiang University Science, 6, 1081-1086.

Viscarra – Rossel R, Walvoort D, McBratney A, Janik L and Skjemstad J, 2006. Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties. Geoderma, 131, 59-75.

Viscarra – Rossel R, McGlynn R and McBratney A, 2006. Determining the composition of mineral-organic mixes using UV-vis-NIR diffuse reflectance spectroscopy. Geoderma, 137, 7-82.

Viscarra – Rossel R, 2007**.** Robust modelling of soil diffuse reflectance spectra by "bagging-partial least squares regression". Journal Near Infrared Spectroscopy, 15, 39-47.

Terhoven-Urselmans T, Schmidt H, Georg Joergensen R, Ludwig, B, 2008**.** Usefulness of near-infrared spectroscopy to determine biological and chemical soil properties: Importance of sample pre-treatment. Soil Biology and Biochemistry, 40, 1178-1188.

Williams P and Norris K, 2001. Near-Infrared Technology in the Agricultural and Food Industries, 2nd Edition. American Association of Cereal Chemist, Minnesota, USA.

World Refrence Base for Soil Resources, FAO, 1998.

Zornoza R, Guerrero C, Mataix-Solera J, Scow K, Arcenegui V and Mataix-Beneyto J, 2008. Near-infrared spectroscopy for determination of various physical, chemical and biochemical properties in Mediterranean soils. Soil Biology & Biochemistry, 40, 1923-1930.