Korean J. Soil Sci. & Fert.(2001)
Vol. 34(4) : 273~277

Possible Use of NIR Spectroscopy for Soil Testing

Kwan-Shig Ryu*, Rae-Kwang Cho**, Woo-Churl Park** and Bok-Jin Kim***

ABSTRACT

Traditional methods of chemical analysis for the soil properties take time and produce harmful waste. The purpose of this research was to evaluate an NIR technique for measuring some soil properties that are rapid and accurate in soil fertility assessments. The NIR instrument (InfraAlyzer 500, Bran & Luebbe Co.) was used for obtaining spectral data from 140 finely ground soil for calibrations and validation estimating pH, CEC, extractable Ca, Mg, K, SiO_2, humic acid and EC. Partial least square regression analysis was used to develop a calibration of NIR spectroscopy method. The results indicated that NIR spectroscopy could be used as a routine nondestructive method quantitatively determining soil chemical properties quickly. However the NIR technique may require sample preparation to obtain even diffuse reflection spectra from the soil and data manipulations to obtain optimal predictions.

Key words : Near infrared (NIR) spectroscopy, Partial least square regression, Diffuse reflectance, Soil analysis, Nondestructive evaluation.

Introduction

Rapid measurement of soil properties has been pursued, e.g. a special technique to analyse many soil samples in a limited time. Present soil testing method for fertilizer recommendation in Korea requires analytical data for pH, organic matter, nitrogen, available phosphorus, CEC, exchangeable Ca, Mg and K. Organic matter and available silicate content refer to nitrogen in paddy soils. Some researchers have shown that the spectra of NIR reflectance contain some information about soil properties(Davis, 1998, Krishnan et al., 1980, Krischenko et al., 1992, Morra et al., 1991, Inoue et al., 1991, Ben-Dor et al., 1995). Kano et al.(1985) have developed a hand held soil moisture meter. Ryu et al.(2000) showed soil analyser for moisture, organic matter and nitrogen using NIR spectroscopy. Ryu et al.(2001) also reported the determination of various extractants soluble phosphorus using NIR spectroscopy. Reeves(1999) and Ryu et al(2001) reported ground soil samples improved a prediction accuracy of soil properties by NIR spectroscopy. Malley et al.(1999) showed good calibration of C, N, clay, CEC, Ca and Mg for Duck Mountain soils and mentioned that NIR spectra was a rapid and cost effective method of soil analysis.

Application of the NIR spectral technique, if sample preparation would improve an accuracy of soil properties, may allow the use for the soil testing method mainly due to

* Department of Agricultural Chemistry, Taegu University.
** Department of Agricultural Chemistry, Kyungpook National University.
*** Department of Agronomy, Youngnam University.
※ This research was partly funded by the Research Grant of Agricultural R & E Promotion Center in Korea..

the simplicity of soil analysis as Meyer(1996) used this technique for fertilizer advisory service. This study was aimed at improving the accuracy of the NIR method to cope with the traditional soil analysis method.

Materials and Methods

Soils

Total of 140 soil samples from paddy, upland, orchard and other land uses subjected to different amounts of soil constituents were collected. Soil samples were ground to pass through 0.2mm opening sieves. 85 soil sample were used for developing calibration and 55 were used for prediction.

Determination of soil properties

The soil pH(1:5) was measured with a glass electrode. CEC was measured by pH 7 of 1N-NH_4OAc method, and Ca, Mg and K extractable by 1N-NH_4OAc and available SiO_2 extractable by 1N-NaOAc was measured by ICP. Humic acid was measured by the international humic subatance society(IHSS) method. EC(1:5) was measured by EC meter(Mettler, MC-226)

NIR spectral measurement of soils

The NIR reflectance spectra for the soils was scanned at 2nm interval from 1,100 to 2,500nm with an InfraAlyzer 500(Bran & Luebbe Co.). Calibration equations were based on a selection of the lowest standard error from the best combination set of several wavelengths with partial least square regression(PLSR) analysis. Standard error of estimation(SEE) and prediction(SEP) were calculated from the following equation.

$SEE = (\text{mean square error})^{1/2}$

$SEP = [\Sigma(x - y)^2 / n-1]^{1/2}$

where x is the soil constituents, y is the predicted value from NIR calibration equations for the soil constituents, and n is the number of samples.

Result and discussion

Ryu et al(2000) and other researcher measured soil moisture, organic matter and total nitrogen using the NIR spectroscopy, and Ryu et al(2001) also measured various fraction of soil phosphorus using the NIR spectroscopy. Figure. 1 shows the various soil properties. These figures explain the relationships between measured data by traditional laboratory methods and predicted data by NIR spectroscopy. Soil pH, extractable Mg, K and SiO_2, and humic acid in soil showed good agreement between measured and predicted value and fell in the vicinity of 1:1 line except for a few outliers, but CEC when more than 15cmol/kg and extractable Ca when more than 2500mg/kg tended to slightly underestimate. EC showed less reliable than other properties due to the large variation.

Partial least square regression procedure between the content of a given constituent and the spectral absorbance of several bands was combined until having the highest coefficient of multiple correlation. Calibrations were evaluated by using the equations to predict moisture, organic matter and total nitrogen for the sample sets that were not used in calibration making.

Bowers and Hanks(1965) observed the particle size effect on reflectance absorbance. Wetzel(1983) explained the influence of particle size and packing pressure of the samples to accommodate the scattering effect as part of the calibration.

In the NIR analysis, the orientation of particles was important in obtaining reproducible NIR reflectance spectral data which allows the interpretation of soil components. Increase of the measuring bands was believed to increase an estimation accuracy of soil properties by obtaining better mean diffuse reflection. Finely ground samples presented successful results for obtaining reproducible reflection for the soil properties and satisfied the pre-treatment conditions for NIR measuring such as even orientation or

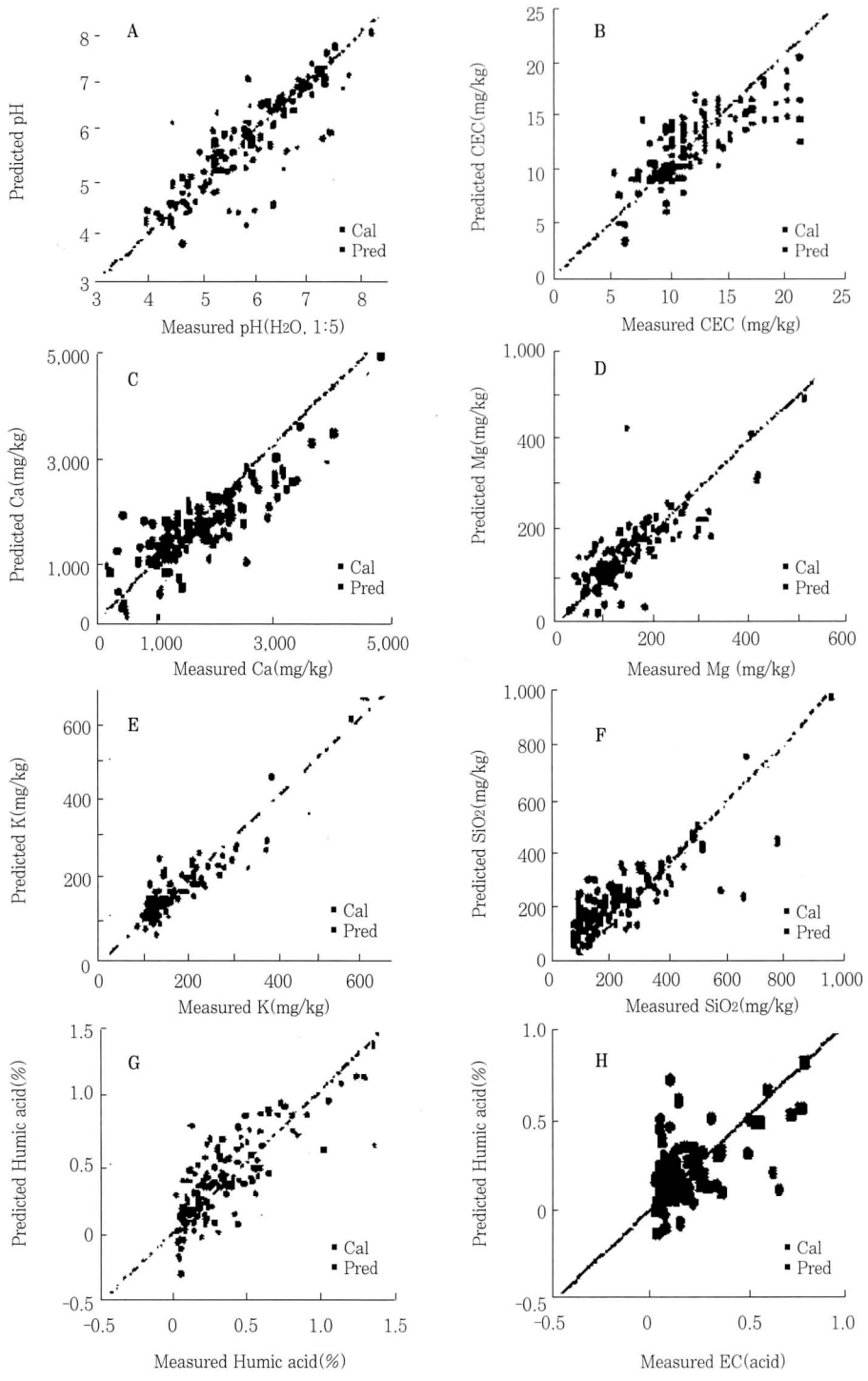

Fig. 1. Relationships between the measured by chemical method and predicted value by NIR method for pH(A), CEC(B), extractable Ca(C) ,Mg(D) and K(E), and available SiO_2(F), humic acid(G) and EC(H) in the soils.

Table1. Results of regression analysis of the soil components for the soils used

soil components	Math	data pretreatment	tern	Soil range	R	SEE	SEP
pH(1:5)	PLSR	2D	9	3.86~8.15	0.972	0.23 (82)	0.82 (53)
CEC(cmol/kg)	PLSR	2D	4	5.0~27.0	0.749	2.60 (84)	2.54 (55)
Ex.Ca	PLSR	2D	6	158.8~5,200	0.901	402.0 (85)	516.5 (54)
Ex.Mg	PLSR	2D	5	23.3~507.8	0.898	39.2 (84)	66.0 (55)
Ex.K	PLSR	2D	7	79.9~602.1	0.947	26.2 (84)	48.2 (53)
Av.SiO5	PLSR	2D	8	37.9~997.7	0.913	74.1 (85)	135.4 (54)
EC(dS/m)	PLSR	2D	8	0.02~2.80	0.979	0.08 (84)	0.21 (51)
humic acid(%)	PLSR	2D	6	0.00~1.91	0.826	0.21 (91)	0.19 (59)

R : Multiple correlation coefficient, SEE : Standard error of estimate,
SEP : Standard error of prediction, ( ) : No. of soil samples
PLSR : partial least square regression, 2D : 2nd derivatives of the spectrum
Term : No. of band used for calibration,

regimentation of soil particles. The wavelength of identifiable bands in the NIR method and the correlation with the soil properties did not show much difference between organic matter and total nitrogen. Table 1 shows the regression analysis of soil properties by NIR method for the finely ground soil samples. Therefore, table 1 explains the scope of the applicability of the NIR method with a reasonable accuracy in routine soil analyses.

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韓土肥誌(2001)
Vol. 34(4) : 273~277

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토양검정에서 근적외 분광분석기의 이용 가능성

유관식* · 조래광** · 박우철** · 김복진***

실험실에서의 기존의 토양분석방법은 많은 시약을 사용하고 분석시간이 많이 걸린다. 본 연구는 근적외 분광분석기를 이용하여 토양의 여러 가지 이화학성분에 대한 측정결과를 검토하였다. 토양시료를 몰탈로 갈아서 토양입자를 0.2mm의 체를 통과시킨 140점의 토양시료를 85점은 근적외 분광분석기(InfraAlyzer 500, Bran & Luebbe Co.)로 표준곡선을 작성하고 나머지 55점의 토양시료는 표준곡선을 이용하여 토양의 이화학성중에서 토양 pH, CEC, 치환성 Ca, Mg, K 및 유효규산, 휴믹산 및 전기전도도(EC)를 추정하였다. 표준곡선은 부분최소자승법을 이용하여 작성하였다. 토양시료를 곱게 분쇄하면 근적외선의 고른 확산반사를 얻을 수 있어서, 근적외 분광분석기를 이용하여 여러 가지 토양의 화학성을 수초내에 추정할 수 있어 토양검정에 이용할 수 있을 것으로 생각된다.

Key words : Near infrared (NIR) spectroscopy, Partial least square regression, Diffuse reflectance, Soil analysis, Nondestructive evaluation.

* Department of Agricultural Chemistry, Taegu University,
** Department of Agricultural Chemistry, Kyungpook National University,
*** Department of Agronomy, Youngnam University,
※ This research was partly funded by the Research Grant of Agricultural R & E Promotion Center in Korea..