바이오시스템공학 (*J. of Biosystems Eng.*)
Vol. 33, No. 4, pp. 260~268 (2008. 8)

광반사를 이용한 한국 논 토양 특성센서를 위한 샘플링과 캘리브레이션 요구조건

이규승 이동훈 정인규 정선옥 Kenneth A. Sudduth

Sampling and Calibration Requirements for Optical Reflectance Soil Property Sensors for Korean Paddy Soils

K. S. Lee D. H. Lee I. K. Jung S. O. Chung K. A. Sudduth

Abstract

Optical diffuse reflectance sensing has potential for rapid and reliable on-site estimation of soil properties. For good results, proper calibration to measured soil properties is required. One issue is whether it is necessary to develop calibrations using samples from the specific area or areas (e.g., field, soil series) in which the sensor will be applied, or whether a general “factory” calibration is sufficient. A further question is if specific calibration is required, how many sample points are needed. In this study, these issues were addressed using data from 42 paddy fields representing 14 distinct soil series accounting for 74% of the total Korean paddy field area. Partial least squares (PLS) regression was used to develop calibrations between soil properties and reflectance spectra. Model evaluation was based on coefficient of determination (R^2), root mean square error of prediction (RMSEP), and RPD, the ratio of standard deviation to RMSEP. When sample data from a soil series were included in the calibration stage (full information calibration), RPD values of prediction models were increased by 0.03 to 3.32, compared with results from calibration models not including data from the test soil series (calibration without site-specific information). Higher R^2 values were also obtained in most cases. Including some samples from the test soil series (hybrid calibration) generally increased RPD rapidly up to a certain number of sample points. A large portion of the potential improvement could be obtained by adding about 8 to 22 points, depending on the soil properties to be estimated, where the numbers were 10 to 18 for pH, 18-22 for EC, and 8 to 22 for total C. These results provide guidance on sampling and calibration requirements for NIR soil property estimation.

Keywords : Calibration, Sampling, Soil sensor, Soil property, Optical reflectance

1. INTRODUCTION

Precision agriculture (PA) is well established in North America, Europe, and Australia, where production fields are relatively large. PA has also attracted interest and seen limited adoption in Asian countries including Korea, where fields are 0.3 to 1.0 ha in size. PA is a management system where application of agricultural chemicals such as fertilizers, pesticides, and herbicides is matched to actual needs point-by-point within fields. This approach can provide economic benefits to farmers and protection of the soil environment from excessive applications of chemicals.

The article was submitted for publication on 2008-7-28, reviewed on 2008-8-7, and approved for publication by editorial board of KSAM on 2008-8-12. The authors are Kyou Seung Lee, Professor, Dong Hoon Lee, Graduate Student, Dept. of Bio-Mechatronics Engineering, Sungkyunkwan University, In-Kyu Jung, Agricultural Researcher, National Institute of Agricultural Engineering, Suwon, Sun-Ok Chung, Full Time Instructor, Chungnam National University, Daejeon, Republic of Korea, and Kenneth A. Sudduth, Agricultural Engineer, USDA-ARS Cropping Systems and Water Quality Research Unit, Columbia, Missouri, USA. Corresponding author: S.O. Chung, Dept. of Bioindustrial Machinery Engineering, Chungnam National University, 220 Gung-Dong, Yusung-Gu, Daejeon, 305-764, Republic of Korea; E-mail <sochung@cnu.ac.kr>.

For successful implementation of PA, site-specific quantification of soil physical and chemical properties affecting soil quality and crop production is important. Many of these properties may change on a finer spatial resolution than can be practically analyzed with laboratory methods due to time and cost of the sampling and analysis procedures. Thus it would be preferable to replace the standard laboratory methods with another approach that would provide accurate characterization of within-field variability at a reasonable cost, and with reliability and timeliness.

Diffuse reflectance spectroscopy (DRS) is a promising, nondestructive technique for rapid analysis of soil physical and chemical properties to fulfill these requirements. Many investigators have successfully estimated soil physical and chemical properties with visible (VIS), near-infrared (NIR), and mid-infrared (MIR) spectroscopy. Total C in arable soils was measured with NIR or VIS-NIR spectroscopy by several researchers (Chang et al., 2001; Confalonieri et al., 2001; McCarty et al., 2002; Mouazen et al., 2007) with r^2 values ranging from 0.73 to 0.95. This technique has also been used to determine organic C in arable soils (Krishnan et al., 1980; Dalal and Henry, 1986; Sudduth and Hummel, 1991; Reeves and McCarty, 2001; Shepherd and Walsh, 2002; Islam et al., 2003; Mouazen et al., 2007) and to estimate soil properties such as cation exchange capacity (CEC), Ca, K, texture (sand, silt, and clay fractions), Mg, pH and total N (Sudduth and Hummel, 1993; Ben-Dor and Banin, 1995; Shepherd and Walsh, 2002; Cozzolino and Moron, 2003; Islam et al., 2003; Nanni and Dematte, 2006).

The DRS approach has also been applied to Asian fields. Shibusawa et al. (2005) developed a real-time multi-spectral soil sensor using nine wavelengths of light. Data collected at 552, 651, 739, 811, 926, 1007, and 1457 nm were used to estimate moisture content (MC) and data at 1303 and 1650 nm were used for soil organic matter (SOM) content. Using partial least squares (PLS) regression, MC was estimated with R^2 of 0.76 and standard error of calibration (SEC) of 2.50% for an Andisol, but SOM was not estimated successfully. Morimoto et al. (2004) used the same sensor body, but different sensing hardware. They collected absorbance spectra from 500 to 1650 nm with a 7 nm interval for 1300 soil samples from Japanese paddy and dryland fields and used those spectra to estimate SOM, total N, pH, and MC. Using a neural network approach, MC, pH, SOM, and total N were estimated with R^2 values of 0.91, 0.75, 0.95, and 0.96, respectively.

One important aspect of DRS estimation of soil chemical and physical properties is identification of the wavelengths or ranges of wavelengths that are strongly related to the soil physical and chemical properties of interest. This is one of the main issues of spectral-based sensing technology, because the success of a calibration model heavily depends on selected wavelength bands (Min and Lee, 2005). In a previous study (Lee et al., 2007) we combined VIS and NIR reflectance sensing using partial least squares (PLS) regression to estimate surface and profile soil properties, and to identify wavelength bands important for estimating soil properties. Soil samples were obtained from 10 fields in five states of the North-Central US. Good estimates of organic C, CEC, Ca, and texture fractions were obtained for both surface and profile datasets. We also applied a similar approach for Korean paddy soils (Chung et al., 2008), and obtained good estimations of Mg (R^2 = 0.80), Ca (R^2 = 0.77), and total C (R^2 = 0.92); fair estimations of pH, EC, P_2O_5, K, Na, sand, silt, and clay (R^2 = 0.59 to 0.72); and poor estimation of total N. In both studies (Lee et al., 2007; Chung et al., 2008), many wavelengths selected for estimation of the soil properties were identical or similar for multiple soil properties. More important wavelengths were selected in the visible-shortwave NIR range (350-1000 nm) and the longwave NIR range (1800-2500 nm) than in the intermediate NIR range (1000-1800 nm).

Other important considerations for a VIS-NIR soil sensor are how many calibration samples are required to provide a prediction model sufficient for field application of the sensor, and how closely the characteristics of those calibration samples must be related to the characteristics of the soils to be analyzed. We investigated these issues for North-Central US soils (Lee et al., 2008) and found that when sample data from a field in question were included in the calibration stage, RPD (the ratio of standard deviation to RMSEP) values of prediction models increased by 0.16 to 1.78 for profile data and 0.02 to 1.58 for surface soil data, compared with results from calibration models that did not include data from the test field. Including some samples from the test field generally increased RPD by 0.7 to 1.5 with 6 to 15 sample points, with little further improvement obtained with additional points.

The overall objective of this study was to apply a similar approach to investigate the sampling and calibration requirements for DRS soil property sensing of Korean paddy soils. Specific objectives were to determine 1) if additional calibration between reflectance and laboratory-determined soil properties would be necessary for application of a sensor under conditions different from those included in its initial calibration, and 2) if so, how many additional sample points from the test area would be required to improve the calibration sufficiently.

2. MATERIALS AND METHODS

A. Soil Sampling and Laboratory Analysis

Soils used in this study were obtained from 39 paddy fields representing 14 distinct soil series that account for 74% of the total Korean paddy field area. Table 1 gives general characteristics of the 14 soil series. Soils of the study areas exhibited differences in parent material, topography, and texture. Texture also varied by depth. For example, in the Sachon series overall texture of the soil profile was sandy loam, but the texture below the A_p horizon (disturbed mineral horizon) was coarse loam (Table 1).

Five 9-cm diameter, 65-cm long sample cores were obtained from each field and segmented by depth on a 5-cm interval. Within each field, soil from each depth was combined and the resulting composite sample analyzed at the Yeongnam Agricultural Research Institute using methods described by the National Institute of Agricultural Science and Technology (2000). P_2O_5 was determined by the Lancaster method, and cations (K, Ca, Mg, and Na) by the ammonium acetate method. Total C, total N, EC, and pH were also determined. The number of samples per soil series varied from 24 (i.e., Bigog) to 52 (i.e., Yecheon) and the total number of samples was 631 (Table 1).

Summary statistics of laboratory measurements are given in table 2. There were wide variations in most of the soil

Table 1 Descriptions of the 14 soil series investigated in this research

Soil series	Parent material	Topography	Overall texture[a]	No. samples
Sachon	Local alluvium from acidic rock	Local alluvial valley	Sandy loam (coarse loam)	52
Chilgog	Alluvium-colluvium from granite	Mountain footslope	Loam (fine loam)	51
Hwadong	Old alluvium	River terrace	Silt loam (fine clay)	39
Maegog	Alluvium-colluvium from acidic rock	Local alluvial valley	Sandy loam (coarse loam)	47
Yecheon	Local alluvium from acidic rock	Local alluvial plain	Sandy loam (coarse loam)	52
Hamchang	Alluvium	Alluvial plain	Sandy loam (coarse loam)	50
Yuga	Local alluvium from gray shale	Local alluvial valley	Silt loam (fine silt)	48
Imgog	Alluvium from acidic rock	Local alluvial valley	Loam (fine loam)	48
Hoegog	Alluvium from acidic rock	Local alluvial valley	Sandy loam (coarse loam)	38
Bigog	Alluvium from acidic rock	Local alluvial valley	Silt loam (fine loam)	24
Gyeongsan	Colluvium from gray shale	Local alluvial valley	Silt loam (fine silt)	52
Gwangpo	Fluvio-marine deposits	Fluvio-marine plain	Sandy loam (coarse loam)	52
Gamcheon	Local alluvium from schist	Local alluvial valley	Loam (Coarse loam)	39
Deunggu	Fluvio-marine deposits	Fluvio-marine plain	Silt loam (fine silt)	39

[a] Texture below A_p horizon given in parentheses

Table 2 Summary statistics of laboratory-determined soil properties

Soil property	Minimum	Maximum	Mean	Standard deviation	Skewness
pH	4.30	8.16	6.23	0.71	-0.17
EC, dS m^{-1}	0.00	2.96	0.41	0.41	2.65
P_2O_5, mg kg^{-1}	0.01	584.32	68.62	104.34	2.87
K, cmol kg^{-1}	0.03	0.82	0.17	0.14	2.48
Ca, cmol kg^{-1}	1.19	22.62	5.52	3.22	1.72
Mg, cmol kg^{-1}	0.30	5.97	1.53	1.14	1.60
Na, cmol kg^{-1}	0.04	1.85	0.25	0.25	3.44
Total C, %	0.12	3.18	0.96	0.68	1.11
Total N, %	0.00	2.68	0.19	0.29	4.23

properties because the samples were from different soil series and depths. For example, P_2O_5 varied from 0.01 to 584.32 mg kg^{-1}. If a single calibration could be developed to represent this variation, we might reasonably expect it to be generally applicable across a wide range of Korean paddy soils in addition to the soils from which it was developed.

B. Spectral Data Acquisition

Soil spectral reflectance data were obtained in the laboratory using an ASD FieldSpec 3[1)] spectrometer (Analytical Spectral Devices, Boulder, Colo.). Spectra recorded between 350 and 2500 nm were output on a 3-nm interval. The spectrometer used three detector systems: 1) a silicon photodiode array for 350-1000 nm, 2) an InGaAs detector for 1000-1800 nm, and 3) an enhanced InGaAs detector for 1800-2500 nm. For reflectance data collection, subsamples of the soils collected in the field were air dried and sieved with a 2-mm screen. Soil was packed in a sample holder with 32-mm inner diameter well and quartz window for reflectance determination. The sample was illuminated through the window by a halogen lamp and the reflected light was transmitted to the spectrometer through a fiber optic bundle. Each soil spectrum was obtained as the mean of 10 scans. The spectrometer data collection software automatically adjusted the data for dark current variations using dark current scans obtained at the beginning of each data collection session, and at least once every 30 minutes thereafter. A Spectralon (Labsphere Inc., North Sutton, N.H.) reflectance standard was scanned after every 10 soils and used to convert the raw spectral data to decimal reflectance.

The reflectance data showed variations for different soil series and depths (Fig. 2). Reflectance data were preprocessed to remove erroneous measurements and improve stability of the regression. The first 30 readings at the lower visible wavelengths were deleted due to their low signal-to-noise ratio, as suggested by Lee et al. (2007). Then, data were transformed from reflectance to absorbance ($\log_{10}$ [1/reflectance]), 1st derivative and normalization were conducted.

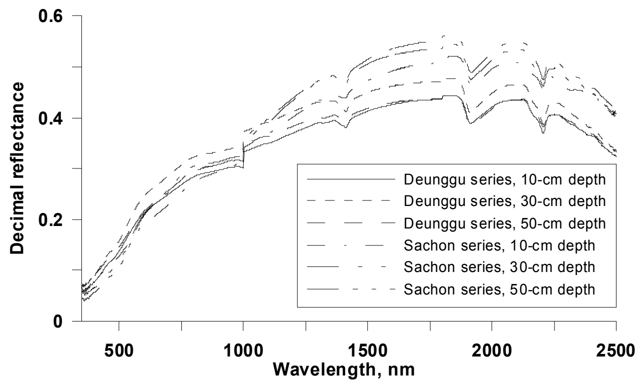

Fig. 1 Soil reflectance spectra for two soil series at three depths.

C. Analytical Procedures

Partial least squares (PLS) regression, implemented in Unscrambler version 9.1 (CAMO Inc., Oslo, Norway), was used to develop calibrations between soil properties and the preprocessed reflectance spectra. PLS has been used widely in chemometrics, remote sensing, and spectral data processing to deal with large numbers of highly correlated variables. PLS creates a new set of variables (called factors) that are uncorrelated and that explain variation in both response and predictor variables (Beebe and Kowalski, 1987). A key step in PLS regression is selecting the optimal number of factors to best represent the calibration data without overfitting. In this analysis, a 10-segment cross-validation approach, an option available in Unscrambler, was used to choose the optimum number of PLS factors.

Model evaluation was based on coefficient of determination (R^2), root mean square error of prediction (RMSEP, eq. 1), and RPD, the ratio of standard deviation to RMSEP.

$$RMSEP = \sqrt{\sum_{i=1}^{n} \frac{(\hat{\gamma}_i - \gamma_i)^2}{n}} \tag{1}$$

where: n = number of samples used for prediction

$\hat{\gamma}_i$ = predicted value of soil property

γ_i = measured value of soil property

RPD is a useful measure of fit when comparing results from datasets containing different degrees of variability, where a higher RPD indicates a more accurate prediction.

1) Mention of trade names or commercial products is solely for the purpose of providing specific information and does not imply recommendation or endorsement by the Rural Development Administration, Republic of Korea, the US Department of Agriculture or their cooperators.

For example, Chang et al. (2001) grouped the ability of NIR spectroscopy to predict values of soil properties into three categories (A, B, C) based on RPD ranges (> 2.0, 1.4-2.0, and < 1.4). In this study, we used increase or decrease in RPD as a main criterion for interpreting differences between prediction models obtained using the different calibration methods described below. Change in R^2 was also used as a secondary criterion.

Data from the 3 to 4 fields in each soil series were pooled for analysis. Three different calibration methods were investigated:

- Method 1: Full Information Calibration. This method used data from all 14 datasets in development of the initial calibration equation. The calibration equation was then used to calculate separate prediction statistics for each of the 14 datasets.
- Method 2: Calibration without Site-Specific Information. This method simulated use of a "factory-calibrated" sensor under conditions different from those used to develop the initial calibration. A calibration model was developed using 13 of the 14 datasets and prediction statistics were calculated for the remaining, "leave-out" dataset. This process was repeated 14 times to obtain prediction statistics for all datasets.
- Method 3: Hybrid Calibration. This method was intermediate between methods 1 and 2, simulating the addition of a small number of specific calibration points to an initial general calibration. PLS calibrations were developed as in method 2, but with a number of additional calibration samples from the "leave-out" dataset included. The number of additional samples was iteratively increased from zero (equivalent to method 2) to the maximum number of points in the dataset (equivalent to method 1). Prediction statistics were calculated as for method 2.

3. RESULTS AND DISCUSSION

A. Method 1 and Method 2

Table 3 shows results of the PLS calibration and cross validation. Reasonable estimates were obtained for all soil properties except total N. Considering both R^2 and RPD criteria, the best estimates were obtained for pH, EC, Ca, Mg, Na and total C.

Table 3 Validation statistics for method 1 soil property estimation using data from 14 soil series in Korean paddy fields

Soil property	Validation R^2	RMSEP	RPD
pH	0.76	0.35	2.04
EC, dS m^{-1}	0.77	0.20	2.08
P_2O_5, mg kg^{-1}	0.72	55.53	1.88
K, cmol kg^{-1}	0.74	0.07	1.95
Ca, cmol kg^{-1}	0.80	1.46	2.21
Mg, cmol kg^{-1}	0.80	0.50	2.26
Na, cmol kg^{-1}	0.76	0.12	2.05
Total C, %	0.95	0.16	4.29
Total N, %	0.02	0.28	1.01

Fig. 2-left is a scatter plot comparing RPD values for soil property estimates by methods 1 and 2. RPD values were located below the 1:1 line, indicating that method 1, where specific soil series information was included, was consistently better than method 2, regardless of soil series or soil property.

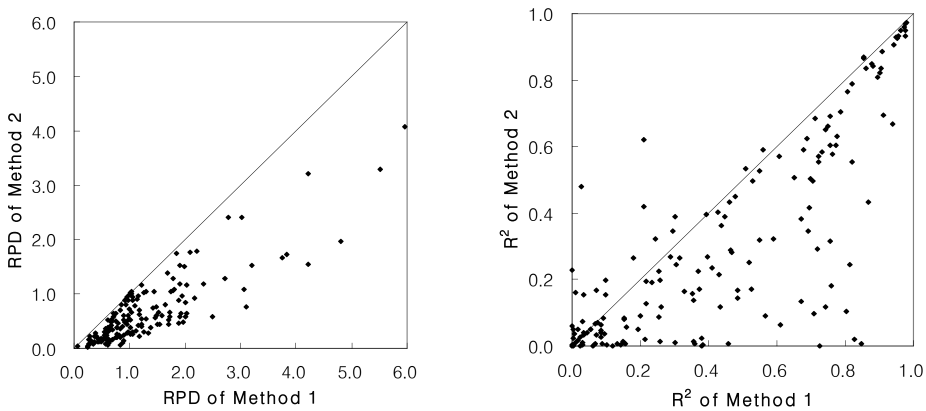

Fig. 2 Comparison of RPD (left) and R^2 (right) statistics for methods 1 and 2 across all datasets. The 1:1 line is also shown for reference.

To further investigate the increase in RPD, method 2 RPD values were subtracted from method 1 RPD values. Soil properties with RPD values greater than 2.0 in the method 1 analysis are shown in table 4. In general, RPD increases varied by “leave-out” dataset and soil property, ranging from 0.03 to 3.32. By “leave-out” dataset (or soil series), average increases were in the range of 1.00 to 1.38 for Hwadong, Maegog, Yuga, and Gamcheon soils. The values were less for the other soils, ranging from 0.36 to 0.91, but they were greater than 0.5, except for Sachon soils, indicating the importance of including soil series-specific information in the initial calibration stage.

RPD increases for total C were generally high with values of 1.68 to 3.32 for Sachon, Hwadong, Yecheon, Hamchang, Yuga, Imgog, Bigog, and Gyeongsan soils, and 0.38 to 0.99 for Chilgog, Maegog, Heogog, Gwangpo, and Gamcheon soils. The mean RPD increase of 1.78 for total C was much greater than that for other soil properties (Table 4). Therefore, it would be particularly important to include calibration soil samples from the specific soil series for total C estimation. Soils with RPD increases greater than 1.00 were Maegog, Yecheon, Hamchang, Yuga, Gamcheon, and Deunggu for pH, Hwadong, Yuga, Gwangpo, and Gamcheon for Ca, and Maegog, Yuga, and Gamcheon for Mg. With this level of RPD improvement, it would be important to include calibration soil samples for all these soil series and soil properties.

Methods 1 and 2 were also compared by calculating increases in R^2 values of method 1 compared to method 2 (Fig. 2, right). These values were mostly positive, indicating that models using method 1 were more predictive than those using method 2 and confirming the RPD analysis. As in the RPD analysis, increases in R^2 values were considerably different for different fields and soil properties.

Based on the RPD and R^2 results, we concluded that NIR soil property estimations would be degraded considerably if sample data from fields with conditions similar to sites where the sensor was to be used were not included in the calibration. The pooled datasets used in this analysis suggested that samples did not need to be from the exact fields under study, but at least should come from fields within the same soil series.

B. Method 3

With method 3, RPD increased as the number of test dataset samples added to the calibration model increased, but degree of the increase was different for different soil series and soil properties. Fig. 3 shows examples of RPD vs. number of sample points added from method 2 for pH (top), EC (middle) and total C (bottom).

Table 4 Difference in RPD values between methods 1 and 2

Soil series	pH	EC	Ca	Mg	Na	Total C	Average
Leave-out dataset							
Sachon	0.63	0.51	0.34	0.18	0.03	2.23	0.65
Chilgog	0.33	0.75	0.19	0.24	0.27	0.38	0.36
Hwadong	0.73	0.72	1.15	0.48	0.80	3.32	1.20
Maegog	1.14	0.82	0.71	1.42	1.49	0.39	1.00
Yecheon	1.10	1.05	0.37	0.19	0.50	1.88	0.85
Hamchang	1.33	0.49	0.67	0.28	0.23	1.68	0.78
Yuga	1.18	0.73	1.20	1.92	0.57	2.67	1.38
Imgog	0.88	0.38	0.90	0.73	0.23	2.34	0.91
Hoegog	0.37	0.41	0.36	0.74	0.67	0.61	0.53
Bigog	0.27	0.29	0.19	0.23	0.09	2.48	0.59
Gyeongsan	0.86	0.44	0.25	0.31	0.31	2.11	0.71
Gwangpo	1.06	0.64	1.37	0.95	0.44	0.98	0.91
Gamcheon	0.48	0.52	2.08	1.43	0.54	0.99	1.01
Deunggu	1.25	0.30	0.48	0.34	0.06	2.84	0.88
Average	0.83	0.57	0.73	0.67	0.45	1.78	

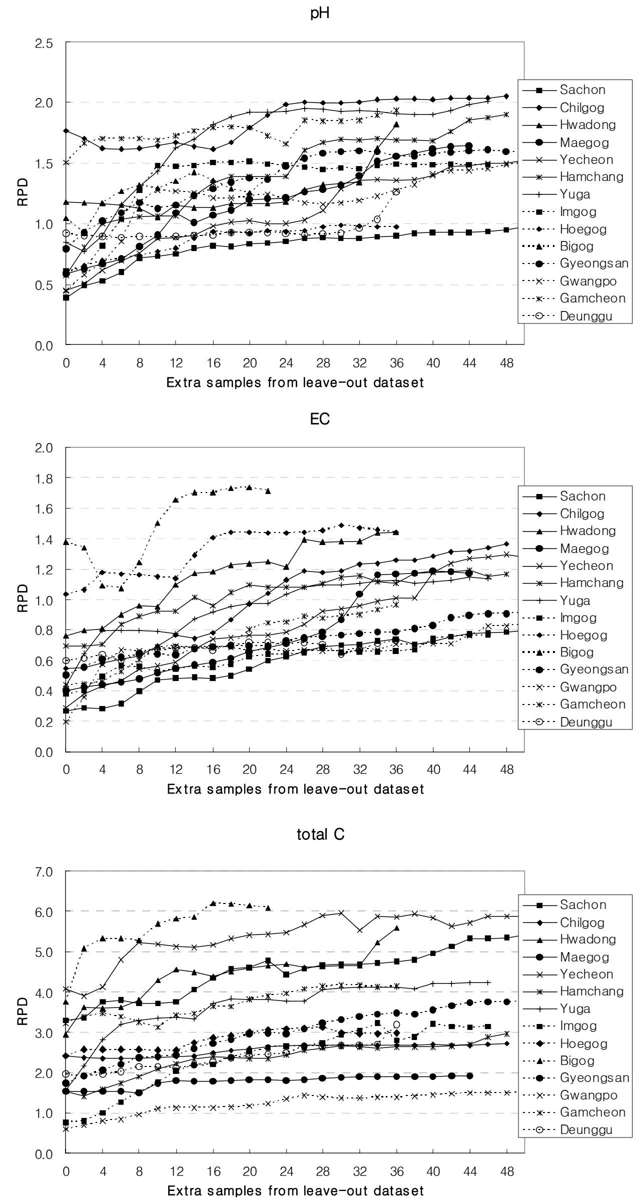

Fig. 3 RPD of calibration model vs. number of sample points included from the "leave-out" dataset for pH (top), EC (middle), and total C (bottom).

For pH, RPD values increased more rapidly as the added points increased up to a certain number (e.g., about 10 for Gwangpo and Imgog, and 18 for Bigog, Yuga, and Hamchang soils), then rate of the RPD increase became lower, and in some cases near zero. RPD increases were about 0.8 and 0.9 with 10 added sample points for Gwangpo and Imgog soils, respectively, and about 1.1 with 18 added points for Yuga soils. For other soils, RPD values increased gradually (e.g., Sachon, Yecheon, and Gyeongsan soils), or there were only slight increases (e.g., Chilgok and Hoegog soils).

For EC, although the slopes of RPD increases were different for different fields, the pattern of RPD increases up to certain numbers (about 18-22) of added points was similar. For total C, initial increases in RPD were greater than for other soil properties. For many soils, the increases were greater than 1.0 with from 8-22 added sample points. For example, the increases were 1.2, 1.5, and 1.9 with 8, 12, and 18 added points for Yecheon, Hwadong, and Yuga soils, respectively.

In general, rates of RPD increase with few added points were greater for soil properties with larger overall increases in RPD between methods 1 and 2 (e.g., total C) than for those with smaller increases (e.g., EC). Most of the improvement in RPD was obtained with a few samples - from 8 to 22 depending on the soil properties to be estimated. Based on these findings, site-specific calibration with a limited number of samples is suggested for accurate results.

4. CONCLUSIONS

The overall objective of this research was to develop a DRS-based soil property sensor for precision agriculture. In this part of the study, different calibration methods were devised and compared to investigate sampling and calibration requirements for the sensor. The data used came from 39 paddy fields representing 14 distinct soil series accounting for 74% of the total Korean paddy field area. Soil samples were obtained on a 5-cm depth interval to a maximum 65-cm depth and analyzed in the laboratory for multiple soil properties. Soil reflectance spectra from 350 to 2500 nm, obtained using a commercial spectrometer, were the dataset used in this study to estimate laboratory-determined soil properties. Major findings were:

- Not including calibration information from a specific soil series (method 2) resulted in lower RPD values compared to including samples from that soil series in the calibration dataset (method 1). Reductions in RPD ranged from 0.03 to 3.32, depending on soil series and soil property. In most cases, R^2 values increased when soil-specific information was added in the calibration stage.
- When the number of soil-specific samples included in the PLS calibration was increased (method 3: hybrid calibration), RPD increased rapidly up to a certain number of added

samples, but the degree of the increase was different for different soil series and soil properties. For many of the soil series, the sample numbers were 10 to 8 for pH (RPD increases of 0.8 to 1.1), 18 to 22 for EC (RPD increases of 0.3 to 0.6), and 8 to 22 for total C (RPD increases of 1.2 to 1.9).

These results provided guidance on sampling and calibration requirements for DRS soil property estimation. Additional data collection, further investigation using additional model selection criteria, interpretation of model improvement in terms of ranges of and DRS responses to each soil property, and automation of these procedures are subjects for future study.

ACKNOWLEDGEMENTS

This research was part of an international joint project, "Development of Site-specific Optimum Soil Management Strategies and In-situ Soil Physical and Chemical Property Sensors for Realization of Environment-friendly Precision Agriculture", between the Rural Development Administration, Republic of Korea and USDA-ARS, USA.

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