Diffuse Reflectance Fourier Transform Mid-Infrared Spectroscopy Associated with Peak Area Integration to Predict Soil Carbonate

Reza Mirzaeitalarposhti[1], Scott Demyan[2], Frank Rasche[3], Georg Cadisch[3], Torsten Müller[4]

[1] Shahid Beheshti University, G.C., Tehran, Iran, [2] Soil and Environmental Mineralogy, The Ohio State University, Columbus, Ohio, USA, [3] Institute of Plant Production and Agroecology in the Tropics and Subtropics, University of Hohenheim, Stuttgart, Germany, [4] Institute of Crop Science, University of Hohenheim, Stuttgart, Germany

A.) Introduction

Soil carbonate is a key component in agricultural soil influencing fertility and productivity. But its determination has need of using labor intensive and expensive traditional approaches. Diffuse reflectance infrared Fourier transform spectroscopy in mid-range (midDRIFTS) has with various degrees of success been used to determine different soil properties. This study evaluated the feasibility of using two different spectroscopic-based approaches, integrated peak area (IPA) & independent calibration (IC), to predict soil carbonate.

B.) Materials and Methods

Soil samples were collected from farmers' fields at 42 locations across two agro-ecological regions [Kraichgau (K) and Swabian Alb (SA); Germany]. A nested sampling design was implemented resulting in a total set of 126 soil samples. Soil samples were analyzed for their carbonate (represented as total inorganic carbon=TIC) using Scheibler's method and also scanned by midDRIFTS. The specific peak area (PA) as an indicator of soil carbonate and composition [e.g. 2515 cm-1 (calcite and dolomite) and 713 cm-1 (calcite)] obtained from midDRIFTS spectra and then were related to carbonate contents separately. Calibration model was also developed via independent calibration (IC) approach taking the whole midDRIFTS spectra via partial least squares regression (PLSR).

C.) Results

➢ **Model development via independent calibration (IC)**

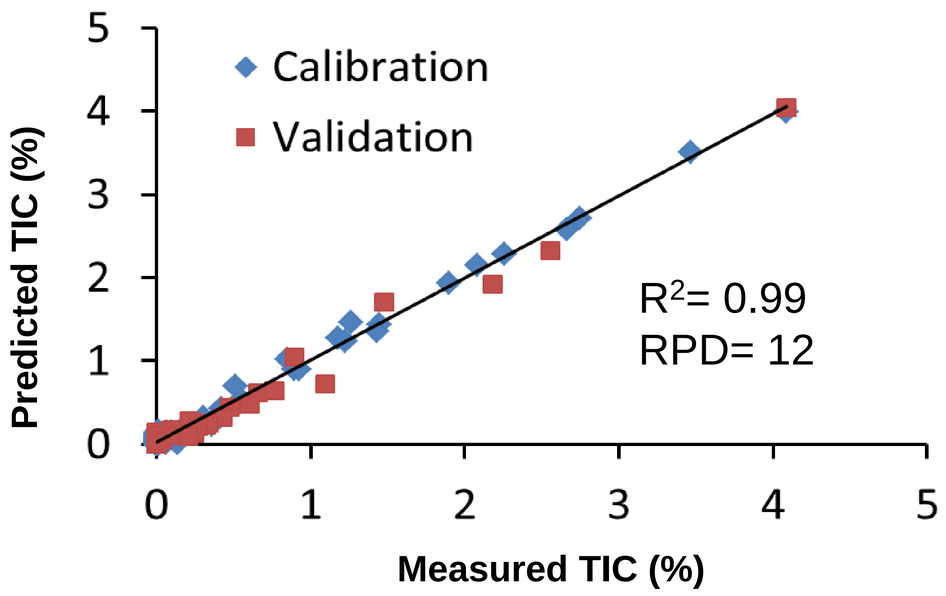

Fig 1. PLSR-predicted vs measured values across both study regions for calibration (n=84) and independent validation dataset (n=42).

➢ **Integrated peak area (IPA) at peaks representing carbonate**

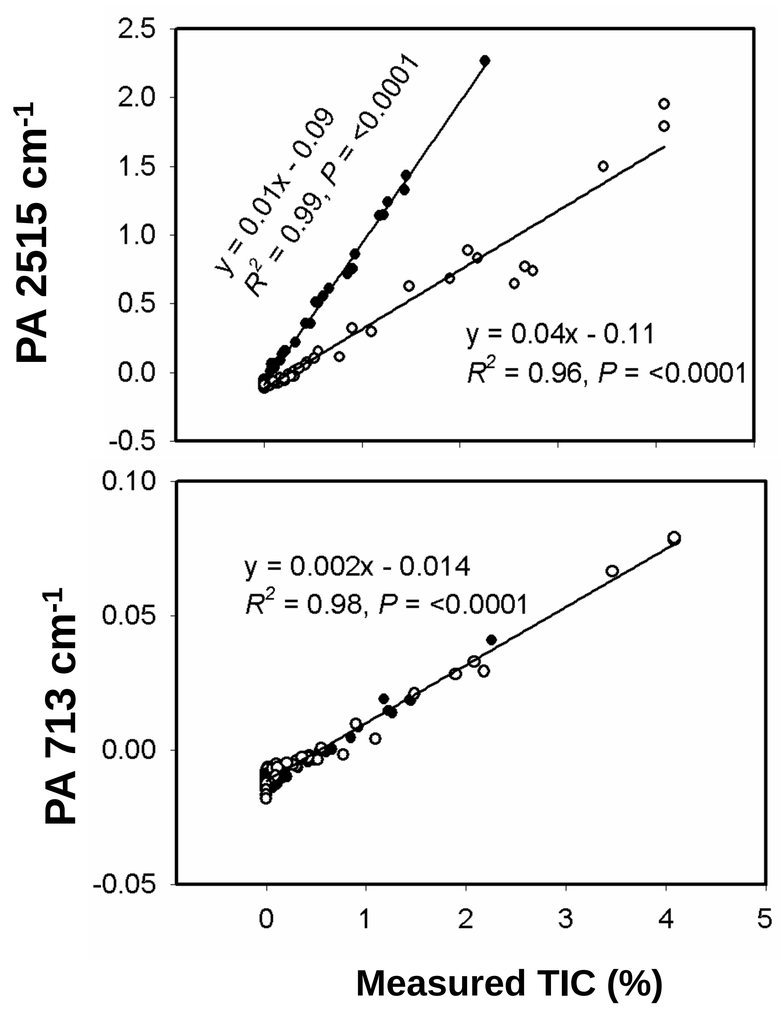

Figure 2. Relationship between TIC and corrected peak area at 2515 and 713 cm^{-1}

D.) Discussion and conclusion

- midDRIFTS-PLSR suggest a significant potential to predict soil carbonate without any further laboratory measurements.
- Spectral data mining resulted in strong correlation between peak area at 2515 cm^{-1} and TIC content but with a divergent trend obtained for each region.
- It was attributed to the error made by presence of dolomite in soils (especially in K soils) which is usually ignored during carbonate measurement by Scheibler's method.
- A strong positive correlation also obtained across both regions indicates the feasibility of bands 713 cm^{-1} to quantify only calcite concentrations in soil.
- The IPA approach for carbonate prediction resulted in a predictive equation as accurate as calibration model developed via IC approach. IPA approach is free of calibration and specifically recommended when the limited number of samples obstacle model calibration via IC approach.

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Contact: Reza Mirzaeitalarposhti ; **rezamirzaei57@gmail.com**