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Improved soil carbonate determination by FT-IR and X-ray analysis

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In forest soils on calcareous parent material, carbonate is a key component which influences both chemical and physical soil properties and thus fertility and productivity. At low organic carbon contents it is difficult to distinguish between organic and inorganic carbon (carbonate) in soils. The common gas-volumetric method to determine carbonate has a number of disadvantages. We hypothesize that a combination of two spectroscopic methods, which account for different forms of carbonate, can be used to model soil carbonate in our study region. Fourier Transform Mid-Infrared Spectroscopy (FT-MIR) was combined with X-ray diffraction (XRD) to develop a model based on partial least squares regression (PLSR). Results of the gas-volumetric Scheibler method were corrected for the calcite/dolomite ratio. The best model performance was achieved when we combined the two analytical methods using four principal components. The root mean squared error of prediction decreased from 13.07 to 11.57, while full cross-validation explained 94.5% of the variance of the carbonate content. This is the first time that a combination of the proposed methods has been used to predict carbonate in forest soils, offering a simple and cheap method to precisely estimate soil carbonate contents while increasing accuracy in comparison to spectroscopic approaches proposed earlier. This approach has the potential to complement or substitute gas-volumetric methods, specifically in study areas with low soil heterogeneity and similar parent material or in long-term monitoring by consecutive sampling.

Reference: Bruckman, V. and K. Wriessnig, Improved soil carbonate determination by FT-IR and X-ray analysis. Environmental Chemistry Letters, 2012: p. 1-6. [DOI:DOI 10.1007/s10311-012-0380-4]