

ANALYTICAL VALIDATION OF A MULTIVARIATE CALIBRATION METHOD FOR DETERMINATION OF SOIL ORGANIC CARBON BY NEAR INFRARED SPECTROSCOPY

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The near infrared diffuse reflectance spectroscopy (NIR - DRS , 700-2500 nm) or NIR - DRS associated with the visible region (Vis/NIR - DRS , 400-780 nm) is considered the most promising analytical technique to replace current routine analysis of soil organic carbon (SOC) due to the numerous advantages of this technique over the traditional ones: it is cheaper, faster, non-destructive and "clean". However, one of the key challenges to enable the implementation of NIR-DRS spectroscopy as a routine method in soil laboratories is to build robust multivariate models from a large number of samples, sufficiently representative of the soil types found in a certain region. In this work, local and global multivariate calibration models were developed and validated for the determination of SOC on a representative set of brasilian soil samples, as well as a critical view of a possible implementation of the NIR-DRS spectroscopy as a routine method of SOC in a near future in all laboratory of soil analysis in Brazil.

The spectral data were preprocessed by Savitzky-Golay's first derivative and the variable selection was made by the variable importance for projection (VIP) method (Andersen and Bro, 2010). The multivariate models were built with PLS regression (Wold et al., 2001) and the outliers detection were performed with a in-house Matlab program by the method described by Martens and Naes (1989).

Martens, H. and Næs, T., *Multivariate Calibration*, John Wiley & Sons, New York, NY, 1989.

Andersen, C.M., Bro, R., 2010. Variable selection in regression-a tutorial. *J. Chemom.* 24, 728–737.

Wold, S., Sjöström, M., Eriksson, L., 2001. PLS-regression: a basic tool of chemometrics. *Chemom. Intell. Lab. Syst.* 58, 109–130.