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Performance comparison of calibration models developed for the prediction of soil nitrogen and carbon contents with various vis-NIR-MIR spectral ranges

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The potential of measurement of key soil properties using visible (vis) and infrared (IR) diffuse reflectance spectroscopy (DRS) has been widely investigated during the last decade. However, limited studies on the effect of spectral range on prediction performance were reported, particularly for the vis, near infrared (NIR) and mid infrared (MIR) spectral ranges. In this study, the performance of calibration models developed for different combinations of spectral ranges, i.e. vis (400-700 nm), vis-short wavelength (SWNIR) (400–1100 nm), NIR (700–2500 nm), vis-NIR (400–2500 nm), ATR-MIR (2500–25000 nm), DRIFT-MIR (2500–25000 nm), vis-NIR-ATR (400–2500–25000 nm), and vis-NIR-DRIFT (400-2500-25000 nm) for the measurement of total nitrogen (TN), total carbon (TC), organic carbon (OC) and inorganic carbon (IC) were conducted using two spectrometers, namely, LabSpec 2500 (ASD Inc. Boulder, CO) with vis-NIR range of 350-2500 nm, and ALPHA Fourier transform infrared (FT-IR) spectrometer (Bruker Optics Inc.) with MIR range of 375-7500 cm^{-1}. A total of 122 soil samples collected from a Silsoe experimental farm, Bedfordshire, The United Kingdom, were divided into calibration (92 samples) and independent validation set (30 sample). Partial least squares (PLS) models were developed based on leave-one-out cross-validation procedure. Results showed that the best PLS model performances were achieved for TN based on ATR spectra with r^2=0.95 and RPD=4.63; for TC based on DRIFT spectra with r^2=0.95 and RPD=4.58, and for OC based on vis-NIR-DRIFT spectra with r^2=0.96 and RPD=6.11. In most cases, PLS models developed for the measurement of TN, TC and OC using DRIFT or vis-NIR-DRIFT spectra outperformed those based on ATR or vis-NIR-ATR spectra, respectively. Although, the prediction of IC was unsatisfactorily, calibration models for IC based on ATR or DRIFT spectra outperformed those built using vis-NIR range or any narrow vis-NIR sub-ranges. It can be concluded that MIR spectroscopy, including ATR and DRIFT, is more suitable for the development of robust PLS models for the prediction of soil N and C, while PLS models based on vis-NIR range or some of narrow vis-NIR sub-ranges, if coupled with relevant spectral pretreatments, also exhibit the potential for excellent PLS modeling of studied soil properties, which is more suitable for practical application in precision farming.