

Calibration and Application of Mid-Infrared DRIFT Spectroscopy for the Analysis of Soil Organic Carbon for different Soil Types and Land Uses in NSW

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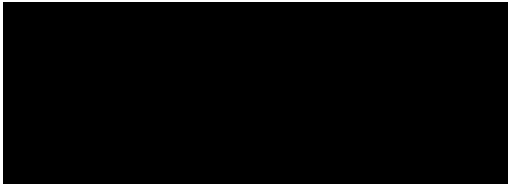
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Certification

I certify that the substance of this thesis has not already been submitted for any degree and is not currently being submitted for any other degree or qualification.

I certify that any help received in preparing this thesis, and all sources used, have been acknowledged in this thesis.



Anthony John Collins

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Abstract

Soil organic carbon is a key indicator of soil condition and health and has attracted considerable research attention due to its potential role in carbon cycling and climate change. This study examined the calibration and application of mid-infrared DRIFT spectroscopy for the analysis of soil total organic carbon (TOC), with the intention of providing the foundation of a calibration model for the State of NSW. The calibration model is intended for use by the Office of Environment and Heritage (OEH) as a cost effective alternative to conventional dry combustion analysis of TOC for the purposes soil condition monitoring. In developing the basis for a State-wide calibration model, a series of individual Soil Monitoring Units (SMUs) and land use calibration models were constructed and compared with all-inclusive global calibration models to estimate and predict TOC. The calibration models were built using 8 SMUs representing distinct soil types and environmental conditions from the NSW State-wide Land and Soil Condition Monitoring, Evaluation and Reporting (MER) program initiated in 2008. The selected SMUs provided a range of different land uses and, where possible, 3 replicates of each land use; cultivation, native pasture and woodland. Soil Monitoring Unit datasets for the soil depths 0-50 and 50-100 mm were used to provide the spectral data and laboratory TOC results.

Individual SMU calibration models and land use calibration models proved to be successful in estimating and predicting TOC. In the estimation of TOC, using the cross validation technique, and in the prediction of TOC of unknown soil samples the calibration models all provided low standard errors of cross validation (SECV) and standard errors of prediction (SEP) values predominantly less than 0.2 with high R^2 0.94 - 0.99. The accuracy of the predicted values were also supported with concordance correlation coefficient ρ_c values close to 1 and residual prediction difference (RPD) values higher than 3. The instances where calibration models gave larger errors in estimating and predicting TOC tended to be the result of a small number of soil samples containing high organic carbon, more than 5% TOC. This may be due to the lack of representation in the calibration datasets used to build the calibration models. These errors were also exaggerated in the back transforming, i.e. the squaring of estimated and predicted TOC values.

When individual SMU calibration models and specific land use calibration models were compared with all-inclusive global calibration models for the same validation datasets their predictive capacities were comparable, yielding similar SEP and R^2 values together with ρ_c and RPD values. Therefore, in the absence of any significant differences in the accuracy to predict TOC it is concluded that all-inclusive global calibration models due to the efficiency of the model would be suitable as the basis of the State-wide calibration model.

In addition to developing calibration models for the analysis of TOC, further investigation was undertaken on the use of mid-infrared DRIFT spectroscopy to estimate organic carbon fractions generated using the CSIRO (Sanderman et al. 2011) and the Zimmerman et al. (2001) fractionation methods both of which have been used in the Rothamsted carbon (Roth C) model. The Roth C model is one of the simpler and more accurate models for simulating the turnover of soil organic carbon (Sanderman et al. 2010). The carbon fraction calibration models were built using the Northern Tablelands Basalts, SMU which provided 9 soil sampling sites for 3 replicates of each land use, cultivation, native pasture and woodland. Composite soil samples were created for the soil depths 0-50 mm and 50-100 mm at each land use sampling site and used to provide the spectral data and laboratory carbon fractions results.

Mid-infrared DRIFT spectroscopy was shown to be reasonably accurate in estimating the CSIRO carbon fraction, particulate organic carbon (POC) with a SECV of 0.27 and R^2 0.83. Calibration models were also built for the Zimmerman et al. (2006) carbon fractions, particulate organic matter (POM), sand and stable aggregate (S + A), silt and clay (s + c) and residual soil organic carbon (rSOC). No model could be produced for the dissolved organic carbon (DOC) fraction due to poor correlation of the mid-infrared spectra with DOC results. The highest accuracy in estimating organic carbon fractions was recorded for the POM fraction with a SECV of 0.08 and R^2 0.74 and rSOC fraction with a SECV of 0.12 and R^2 of 0.79.

In conclusion, OEH, now has the foundation of a State-wide calibration model that can be developed with further inclusion of other SMUs from the MER program into a comprehensive calibration model for the analysis of TOC. This resource would allow OEH to efficiently analyse large number of soil samples for TOC with the potential use of measuring changes in soil organic carbon across the State for the purpose of monitoring soil condition and potentially change in soil organic carbon resulting from management or time.