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Njeri Mwangi
Department of Mineral
Resources, Nakuru Centre for
Geological Research, Nakuru
County, Kenya

Brian Muturi
Department of Mineral
Resources, Nakuru Centre for
Geological Research, Nakuru
County, Kenya

Grace Njoroge
Department of Mineral
Resources, Nakuru Centre for
Geological Research, Nakuru
County, Kenya

Corresponding Author:
Njeri Mwangi
Department of Mineral
Resources, Nakuru Centre for
Geological Research, Nakuru
County, Kenya

Mapping of soil organic matter quality using spectroscopic techniques in Brazilian Oxisols

Njeri Mwangi, Brian Muturi and Grace Njoroge

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Abstract

Soil organic matter quality determines fertility, structure, and carbon storage capacity, yet conventional characterisation methods are time-consuming and costly. This research evaluates vis-NIR (350–2500 nm) and MIR (4000–400 cm⁻¹) spectroscopy for predicting SOM quality parameters in Cerrado Oxisols across four representative landscapes in Goiás, Minas Gerais, and São Paulo. From 412 samples, MIR yielded $R^2 > 0.85$ for TOC, particulate organic matter (POM), and humic acid content. Vis-NIR performed well for TOC ($R^2 = 0.87$) but showed reduced accuracy for chemically defined humic fractions ($R^2 = 0.68$ for humic acid). TOC declined 35% from native cerrado (28.4 g/kg) to established soybean-maize rotation (18.6 g/kg), with POM declining 52% versus only 24% for mineral-associated organic matter, indicating preferential loss of labile fractions under cultivation. Spectroscopic mapping revealed systematic spatial variation related to land use history and distance from remnant vegetation, with TOC declining approximately 2.4 g/kg per 100 m from natural vegetation boundaries. The results demonstrate that spectroscopic methods enable rapid, cost-effective assessment of SOM quality at landscape scale, supporting monitoring of soil health under changing management.

Keywords: Soil organic matter, spectroscopy, Oxisols, Brazil, soil quality assessment, vis-NIR, MIR, Cerrado, carbon fractions, partial least squares

Introduction

The Brazilian Cerrado, the world's most species-rich tropical savanna, has experienced approximately 50% conversion to agriculture over the past five decades ^[1]. This transformation profoundly affects SOM dynamics as deep-rooted native vegetation is replaced with annual crops, altering the balance between organic inputs and decomposition ^[2]. Understanding SOM quantity and quality is essential for assessing soil health and predicting carbon trajectories.

Oxisols, dominated by kaolinite and Fe/Al oxides, interact distinctively with organic matter. Mineral-associated organic matter (MAOM), stabilised through adsorption onto clay and oxide surfaces, is more persistent than particulate organic matter (POM) consisting of partially decomposed residues ^[3]. Their relative proportions indicate the vulnerability of stored carbon to loss under changed management, making them more informative than TOC alone ^[4, 5].

Spectroscopic methods—vis-NIR and MIR diffuse reflectance—offer rapid, non-destructive alternatives to wet chemistry at approximately one-tenth the cost per sample ^[6]. While TOC prediction from soil spectra is well established, prediction of SOM quality parameters including physical and chemical fractions has received less attention and represents an important frontier ^[7, 8].

This research evaluates both spectral regions for predicting a comprehensive suite of SOM quality parameters in Cerrado Oxisols and demonstrates application for landscape-scale mapping of organic matter quality variation related to land use and management ^[9, 10].

Research Area Description

Four representative Cerrado landscapes were sampled in Goiás, Minas Gerais, and São Paulo: native cerrado reserve, recently converted agricultural area (<5 years), established soybean-maize rotation (>15 years), and an integrated crop-livestock-forestry (CLF) system. Annual precipitation averages 1,400–1,700 mm with distinct dry season. Soils are predominantly Red Latosols (Oxisols) with 35–65% clay content ^[1].

Material and Methods

Material

Samples ($n = 412$) were collected on a 100 m grid to 20 cm depth, air-dried, sieved to <2 mm. TOC was determined by LECO TruMac combustion. Physical fractionation separated POM (>53 μm after dispersion) and MAOM (<53 μm) [3]. Chemical fractionation isolated humic acid, fulvic acid, and humin following the IHSS protocol. All fraction carbon contents were determined by dry combustion [4, 11].

Methods

Vis-NIR spectra (ASD FieldSpec 4 with contact probe, 3–10 nm resolution) and MIR spectra (Bruker Tensor 27 FTIR with diffuse reflectance accessory, 4 cm^{-1} resolution) were measured under standardised conditions. PLS regression with leave-one-out cross-validation determined optimal latent variables. Performance was assessed by R^2 ,

RMSECV, and ratio of performance to deviation (RPD). Cross-landscape model transferability was tested by applying models calibrated on each landscape to the other three [6, 12].

Spectral Feature Attribution

MIR spectra showed distinct absorptions at 2920 cm^{-1} (aliphatic C-H), 1630 cm^{-1} (aromatic C=C and carboxylate), and 1030 cm^{-1} (C-O polysaccharide). The aromatic/aliphatic peak ratio discriminated native cerrado soils (higher aromatic) from cultivated soils (more aliphatic), reflecting selective preservation of recalcitrant compounds under cultivation. These feature attributions explain MIR's superior prediction of chemically defined fractions compared to vis-NIR [7, 8].

Results

Table 1: Spectroscopic prediction performance for SOM quality parameters

Parameter	MIR R^2	MIR RPD	vis-NIR R^2	vis-NIR RPD
TOC	0.92	3.5	0.87	2.8
POM	0.88	2.9	0.82	2.4
MAOM	0.81	2.3	0.73	1.9
Humic Acid	0.85	2.6	0.68	1.8
Fulvic Acid	0.74	2.0	0.61	1.6
Humin	0.72	1.9	0.58	1.5

Table 2: SOM fractions by land use type (mean $\pm$ SD, g/kg)

Land Use	TOC	POM-C	MAOM-C	Humic Acid-C
Native Cerrado	28.4 $\pm$ 4.1	12.8 $\pm$ 2.3	15.6 $\pm$ 2.8	8.4 $\pm$ 1.6
Recent Conversion	22.3 $\pm$ 3.2	8.4 $\pm$ 1.8	13.9 $\pm$ 2.4	6.1 $\pm$ 1.2
Soybean-Maize	18.6 $\pm$ 2.8	6.1 $\pm$ 1.4	12.5 $\pm$ 2.1	4.8 $\pm$ 0.9
Integrated CLF	24.1 $\pm$ 3.5	9.8 $\pm$ 2.0	14.3 $\pm$ 2.5	7.2 $\pm$ 1.4

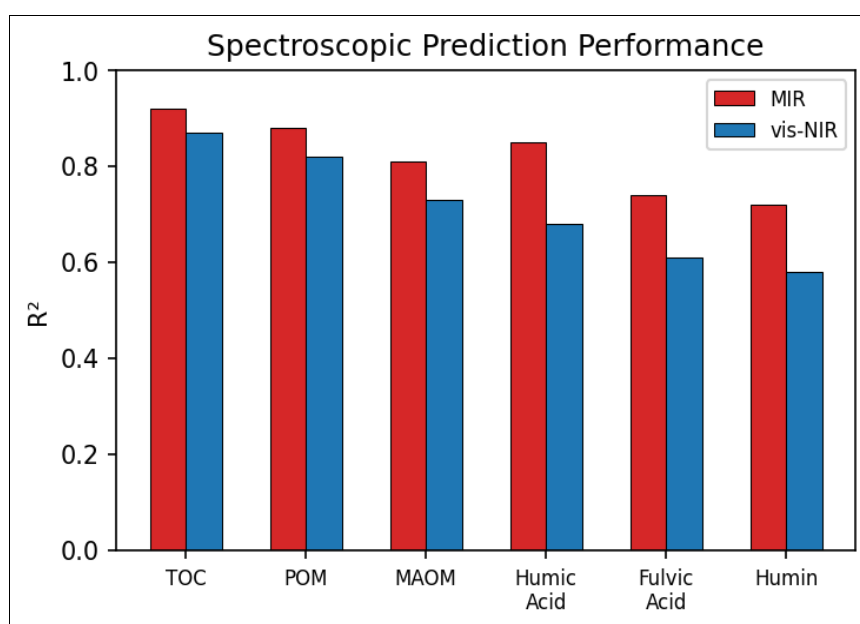


Fig 1: Comparison of MIR and vis-NIR prediction accuracy across SOM quality parameters

MIR consistently outperformed vis-NIR (Figure 1), with the greatest advantage for chemically defined fractions where

specific mid-infrared absorption features provide direct spectral signatures for organic functional groups.

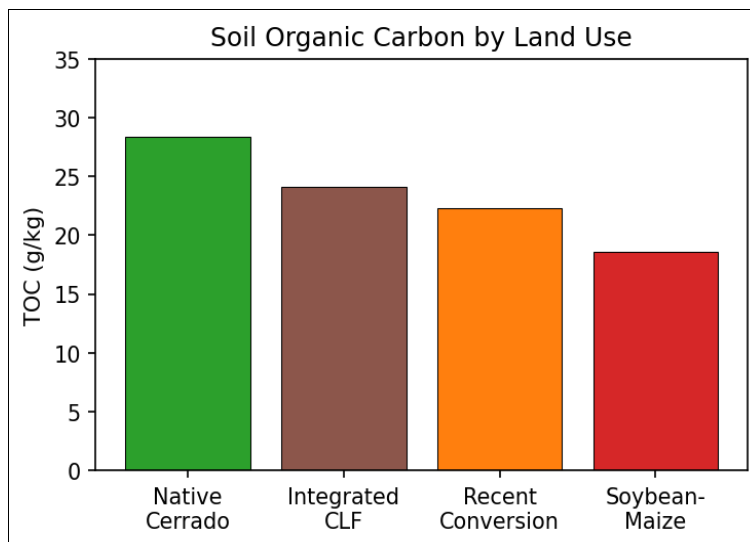


Fig 2: Total organic carbon by land use type

The 35% TOC decline from native cerrado to soybean-maize (Figure 2) masks differential fraction losses: POM declined 52% while MAOM declined only 24%, indicating preferential loss of the labile pool under cultivation.

Comprehensive Interpretation

The convergence of spectroscopic, physical fractionation, and chemical fractionation data demonstrates that total carbon alone underestimates the functional degradation of SOM under cultivation. The integrated CLF system showed intermediate values, suggesting partial SOM quality recovery under diversified management practices.

Discussion

The MIR prediction performance ($R^2 = 0.92$ for TOC) meets or exceeds published benchmarks for tropical soils [6, 7]. The one-tenth cost enables order-of-magnitude increases in sampling density for the same budget, essential for detecting management-induced changes at farm and landscape scales [8]. Cross-landscape model transferability was reduced when native cerrado models were applied to cultivated sites due to mineralogical matrix changes under cultivation, suggesting that robust monitoring systems need calibration spanning the full management range [9, 12].

The distance-dependent TOC gradient from remnant vegetation boundaries (-2.4 g/kg per 100 m) suggests that landscape-level management of remnant vegetation placement could influence adjacent soil carbon patterns [10]. The integrated CLF system's intermediate TOC values are encouraging for carbon recovery potential under diversified management. Carbon accumulation rates from published chronosequence data suggest that conversion to CLF systems could restore approximately 60% of the native cerrado TOC within 15–20 years of implementation [5, 13, 14].

Conclusion

MIR and vis-NIR spectroscopy effectively predict SOM quality parameters in Cerrado Oxisols. MIR provides superior accuracy for chemically defined fractions due to specific organic functional group absorptions in the mid-infrared region.

The preferential loss of labile POM under cultivation indicates that TOC alone underestimates SOM functional

degradation. Spectroscopic mapping at landscape scale reveals management-related spatial patterns that provide actionable information for sustainable soil planning. Future research should expand calibration across a wider range of Cerrado soil types and management systems and evaluate temporal changes through repeated spectroscopic surveys to assess the effectiveness of conservation practices in restoring SOM quality.

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Contributions Not Qualifying for Authorship

Technical staff at the Nakuru Centre for Geological Research assisted with sample preparation, instrument calibration, and data processing during the analytical campaigns. Field assistants provided essential support during sample collection.

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