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Potential of Mid-Infrared Spectroscopy as Complementary Technique for Assessment of Soil Engineering Properties

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Abstract

Mid-infrared (MIR) spectroscopy has emerged as a rapid and cost effective complementary to conventional laboratory methods utilized for assessing soil properties. The study intends to evaluate the potential of MIR spectroscopy for non-destructive estimation of some engineering soil properties along Ilorin – Kabba expressway. Fifty georeferenced soil samples from different Basement Complex rock of Southwestern Nigeria were subjected to Fourier-Transform-Infrared-Spectrometric (FTIR) analysis within the spectral region ranging from 4000 – 400 cm^{-1} of electromagnetic radiation. Four preprocessed filtering methods such as moving average, normalization, multiplicative scatter correction, Savitzky-Golay (SG) first derivative algorithm were applied in the pre-treatment of spectral information. Partial Least Squares Regression (PLSR) was employed to develop calibration models for soil properties, with model performance assessed using the coefficient of determination (R^2), root mean square error (RMSE) and ratio of performance to deviation (RPD). The results showed that MIR spectroscopy effectively estimated the properties including sand and clay content, liquid limit, plasticity index, optimum moisture content, maximum dry density, and soaked California Bearing Ratio, achieving an average R^2 of 0.6, RMSE of 1.32, and RPD of 2.1. This study demonstrates the capability of MIR spectroscopy as a rapid and efficient tool for simultaneous estimation of multiple soil properties relevant for engineering purposes. Further research is recommended using diverse non-parametric data mining techniques to enhance soil predictive accuracy.

Keywords: *MIR spectroscopy, FTIR spectroscopy, Index properties, PLSR, Coefficient of Determination, RPD.*

Introduction

Soil is composed of minerals, organic matter, micro-organisms, air, and water, serving as a vital resource for infrastructure development, agricultural productivity, and ecosystem functioning, whose detailed information is highly sought after by engineers and policymakers. The most essential parameters in geotechnical engineering are the soil moisture content, plasticity index, cohesion, unit weight, grain size distribution, porosity, etc. These properties are important in determining bearing capacity and slope stability of soil. However, they are tedious, relatively expensive, time-consuming and require experienced skilled operators with large amount of soil materials as specimen. Various tests deployed to provide rapid indicators of soil functional capacity during preliminary engineering investigations include particle size analysis, consistency limits, linear shrinkage, moisture content, density, California Bearing Ratio (CBR), etc. Consistency limits, in particular, was reported by Sridharan (2014) to correlate strongly with critical soil properties such as shear strength, compressibility and permeability. However, conventional methods are often expensive, time-consuming, invasive, and involve the physical destruction of the soil system (Mousavi *et al.*, 2021). Therefore, there is a need for a fast, non-destructive, and reliable method for the rapid estimation of soil properties.

Advanced spectroscopic techniques are increasingly being utilized to predict soil engineering properties. Among these, visible and near-infrared (VNIR: 25,000 - 4,000cm^{-1}) and mid-infrared (MIR: 4,000 - 400cm^{-1}) spectroscopy are the most commonly applied spectral regions for soil analysis (Viscarra Rossel *et al.*, 2006). Both techniques are rapid, non-destructive, and simple, enabling the simultaneous inference of multiple soil properties from a single spectral scan. These attributes make VNIR and MIR spectroscopy particularly suitable for high throughput analysis and in situ applications. VNIR and MIR are vibrational spectroscopy methods, which relies on the absorption of electromagnetic energy through various molecular vibrational modes (Fig. 1). The MIR region captures fundamental vibrational absorption bands that are strong, distinct, and capable of fingerprinting specific chemical bonds. In contrast, the VNIR region detects weaker, overlapping overtones of these bands.

Several studies have demonstrated the application of these techniques to estimate soil engineering properties,

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including clay content, Atterberg limits, swelling potential, California Bearing Ratio (CBR), and unconfined compressive strength (Mousavi *et al.*, 2020, 2021; Yitagesu *et al.*, 2009; Waruru *et al.*, 2014; Tian *et al.*, 2013; Soriano-Disla *et al.*, 2014). These findings highlight the potential of spectroscopic techniques as efficient tools for soil property assessment.

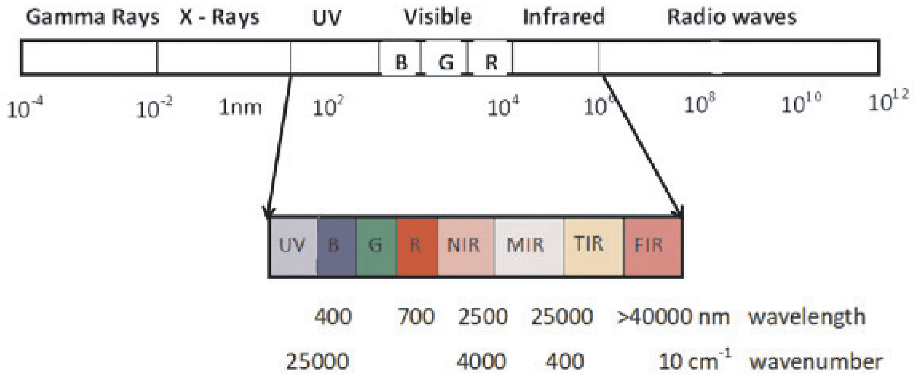

Fig. 1: The electromagnetic spectrum showing the infrared region (McBratney et al., 2003)

Mousavi *et al.* (2019) used PLSR combined with back propagation of neural network (PLS-BPNN) to develop empirical prediction models for estimating Atterberg limits and unconfined compressive strength (UCS) from soil reflectance spectra. Their results demonstrated a strong potential for spectroscopy in soil property estimation. Similarly, Tian *et al.* (2013) analyzed two-band combinations of soil spectral indices such as difference and ratio indices, using linear and non-linear regression techniques to estimate soil organic content. Their findings indicated superior predictive accuracy using PLSR and PLS-BPNN models. Soriano-Disla *et al.* (2014) hypothesized that MIR spectroscopy is more effective in estimating clay and sand contents than silt content due to the distinct fundamental vibrations associated with specific minerals. For instance, clay minerals such as kaolinite (3690–3620 cm^{-1}), smectite (3630–3620 cm^{-1}), and illite (3400–3300 cm^{-1}) exhibit well-defined absorption bands, as does quartz in sand (1100–1000 cm^{-1}). In contrast, silt comprises a variety of minerals with multiple functional groups, resulting in complex vibrations and overlapping peaks that hinder accurate prediction.

Sophisticated statistical approaches are essential for quantitative spectral analysis of soils using reflectance spectroscopy, which links soil attributes to their spectral responses. Various chemometric methods have been applied to mathematically extract information from preprocessed spectral data and empirically relate it to conventional laboratory measurement to develop MIR calibration models (Viscarra Rossel *et al.*, 2006; Xia *et al.*, 2018). Robust prediction models for different soil properties require MIR spectra to undergo calibration and independent validation with laboratory analyzed data. While several studies have explored the use of MIR-diffuse reflectance spectroscopy to predict soil properties, no research has focused on using MIR spectroscopy combined with chemometrics to predict engineering soil properties within the Nigerian subcontinent. This study was conducted to evaluate the potential of MIR spectroscopy for estimating key soil engineering properties – sand and clay content, plasticity, optimum moisture content (OMC), maximum dry density (MDD), and soaked California Bearing Ratio (CBR) from soil samples along the Ilorin-Kabba expressway in Southwestern Nigeria. The specific objectives were to assess the potential of MIR spectroscopy as a rapid, cost-effective tool for estimating soil properties, identify spectral regions with high explanatory value for predicting these properties based on the calibration information and compare the accuracy of the resulting prediction models. This study addresses a critical gap by integrating MIR spectroscopy and chemometrics to evaluate engineering soil properties in a region with limited prior research in this area.

Study Location

The study area is the Ilorin – Kabba highway, located between latitude 7°25'N and 8°40'N and longitude 4°30'E and 6°45'E (Fig. 2).

The region features a low to moderately high elevation ranging from 200 to 800 meters above mean sea level,

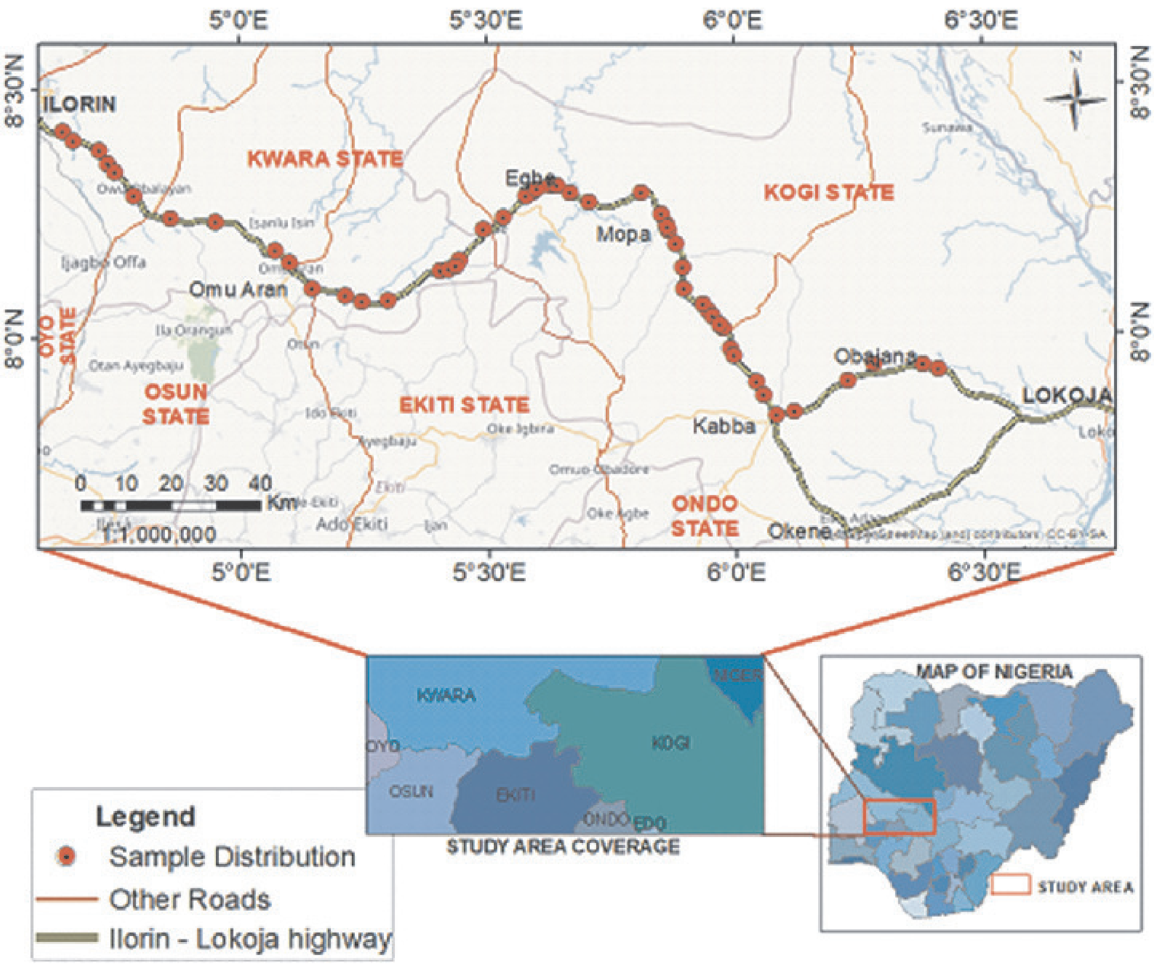

Fig. 2: Map showing the studied highway (inset: bounded states extracted from Nigeria map)

with temperatures varying between 25° and 35°C, and a mean annual rainfall of approximately 1200 mm. This 240-kilometer-long highway is underlain by the Basement Complex rocks of Southwestern Nigeria. The geology comprises three heterogenous lithologic units: the migmatite - gneiss complex, meta-sediments / volcanic rocks, and the older granite series (Fig. 3). These lithologic variations significantly influence the soil patterns observed across the highway.

Materials and Methods

Soil sampling

A total of 50 georeferenced soil samples were randomly collected along the highway corridor, covering three lithologic units: migmatite - gneiss complex, meta-sediments / volcanic rocks, and older granite series (Fig. 3). The migmatite-gneiss complex, predominantly underlying the highway, consists of migmatite, banded gneiss, flaggy quarzite with biotite gneiss, undifferentiated schists, porphyritic granite (porphyroblastic), and medium to coarse-grained biotite and hornblende granite. Soil samples were collected from depths of 0.8 – 1.5m from both stable and failed portions of the highway. Before laboratory analyses, the samples were air-dried at a controlled temperature of 30 – 35°C for two weeks to stabilize moisture content and then gently sieved through a 2 mm mesh to remove coarse particles.

Geotechnical Laboratory Analysis

Geotechnical laboratory tests were conducted based on BS 1377: 1990 standard method to determine grain size distribution, consistency limits, optimum moisture content, maximum dry density and California Bearing Ratio. Soil compaction was carried out using Modified Standard Proctor method. Soil activity was calculated based on Skempton's (1953) definition, which is the ratio of plasticity index to the percentage of clay content. The soils were classified according to the

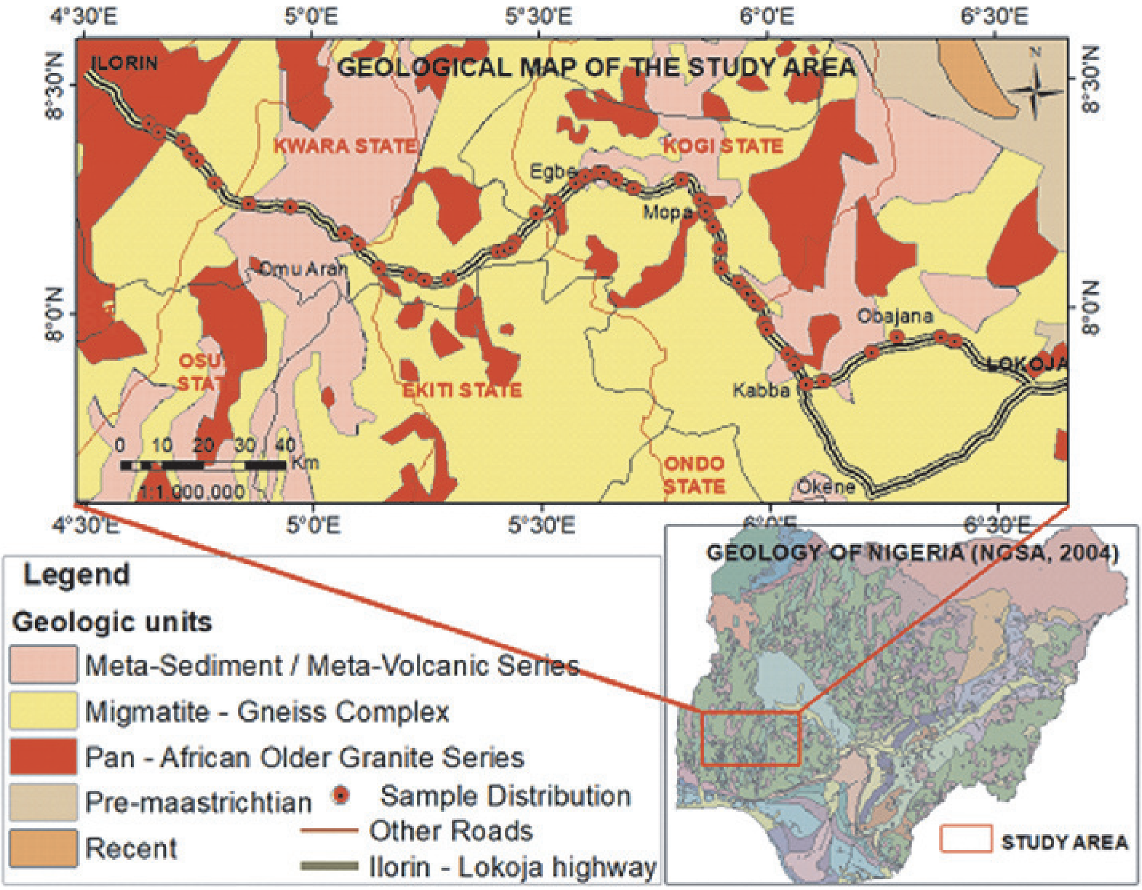

Fig. 3: Sample location developed over three geological units (Source: NGSA, 2004).

Unified Soil Classification System (USCS) to categorize their engineering properties and behaviour.

MIR Spectral Measurements of Soil Samples and Preprocessing of Soil Spectra

For MIR scanning, 10 mg of the same soil portion was finely ground to approximately 0.07 mm particle size at 105°C and analyzed using a Bruker Vertex 70 Fourier Transform Infrared (FTIR) Reflectance spectrophotometer. The spectral range spanned from 4000 cm^{-1} – 400 cm^{-1} with a resolution of 2 – 4 cm^{-1} and an accuracy of ±4 cm^{-1}, conducted at the Department of Chemical Sciences Laboratory, University of Johannesburg, Doornfontein Campus, South Africa. A reference cap was scanned to generate a background spectrum, which provided a baseline for the instrument's no-sample condition. Three scans (each with ten successive spectra) were collected for each soil sample and averaged to produce a single spectrum, which was stored in the Optics Users Software (OPUS) file format for further analysis, in line with the international standard described by Shepherd (2010).

The averaged spectral data were converted into CSV format for spectra pre-treatment to reduce noise and enhance signal clarity, especially in the noisy 700 – 400 cm^{-1} spectral regions. Afterwards, several preprocessing algorithms were applied to enhance the spectral data, including moving average, normalization, multiplicative scatter correction, Savitzky-Golay (SG) first derivative algorithm (Gholizadeh *et al.*, 2014). After several trials, maximum normalization using the extended multiplicative signal correction (EMSC) was found to best fit the spectral data (Kohler *et al.*, 2005).

Soil mineral abundances were analyzed by isolating spectra in specific wavelength ranges to enhance the identification of absorption features for each mineral. These ranges included 400 – 1200 cm^{-1}, 1200 – 1800 cm^{-1}, and 2800 – 4000 cm^{-1}. The analysis focused on identifying diagnostic features for phyllosilicate minerals (such as kaolinite, illite, smectite), and non-phyllosilicate minerals (including quartz, hematite, microcline), as well as organic carbon, carbonate and water. The relative abundance of each mineral was determined by calculating the diagnostic absorption peaks in eight specific spectral ranges: 425 – 500 cm^{-1}, 530 – 715 cm^{-1}, 770 – 920 cm^{-1}, 1000 – 1415 cm^{-1}, 1630 – 1700 cm^{-1}, 2830 – 2935 cm^{-1}, 3220 – 3430 cm^{-1}, 3620 – 3700 cm^{-1}. To eliminate interference from CO_2, the CO_2 absorption bands in the 2200 - 2400 cm^{-1} regions were excluded from the analysis. This selection of optimal spectral features, as documented by several studies (e.g., Xing and Chen, 2013), aimed to eliminate non-informative variables, thereby improving the predictive capability and reducing the complexity of the calibration model.

Chemometric and Validation Analyses

As described by several researchers (e.g., Wold *et al.*, 2001; Wijewardane *et al.*, 2018), partial least square regression (PLSR) was used to establish relationships between soil variables and spectra due to its ability to manage multi-collinearity among predictors. The analysis was implemented in R (version 4.0) (RStudio, 2020). Given the limited number of samples, a leave-one-out cross-validation (LOOCV) procedure was applied to calibrate and validate the PLSR model. In this method, for each iteration, *n*-1 samples were used to build the regression model, and the soil property of the excluded sample was predicted using the model. This process was repeated for all *n* samples, generating predictions for all the samples in the dataset. To identify and remove outliers in the calibration set, the Mahalanobis distance method was applied to ensure that only reliable data was used in model development.

The accuracy of the soil properties prediction models was evaluated using three parameters: the coefficient of determination of cross-validation (R^2) (Equation 1), the root mean squares error of cross-validation (RMSE) (Equation 2), and the ratio of performance to deviation (RPD) (Equation 3). Chang *et al.* (2001) categorized RPD into three classes where category A ($RPD > 2$) describes models with high accuracy for predicting soil properties; category B ($2 > RPD > 1.4$) describes models with limited predictive power and category C ($RPD < 1.4$) describes models with no predictive ability. Additionally, Towett *et al.* (2015) suggested that models with $R^2 \geq 0.70$ and RPD ≥ 2 are considered to have good accuracy levels for soil prediction; $R^2 = 0.6$ to 0.7 and RPD = 1.4 to 2.0 provide satisfactory or moderate predictions while lower RPD values indicate poor prediction performance.

$$R^2 = 1 - \frac{SS_{error}}{SS_{total}} \quad \ldots\ldots\ldots\ldots\ldots\ldots 1$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=0}^{n}\left(y_i - y_p\right)^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots 2$$

$$RPD = \frac{SD}{RMSE} \quad \ldots\ldots\ldots\ldots\ldots\ldots 3$$

n - total number of observations;
y_i - observed value;
y_p - estimated value;
SS_{error} - sum of squared errors between estimated and observed values;
SS_{total} - sum of squared deviations of each response variable from its mean;
SD - standard deviation

Results and Discussions

Geotechnical properties of soils

Descriptive statistics of geotechnical properties of the 50 soil samples are summarized in Table 1, showing significant variability in the percentages of sand (≥ 0.075mm), silt (0.002mm) and clays (0.001mm) across the three lithologic units. Sand content ranges from 44% – 81% with a mean of 60.7%. A higher proportion of fines (silt and clay) is observed in the migmatite gneiss (MGR) unit, ranging from 10% – 68% with a mean > 20%, and in the meta-sediment/volcanic (MSVR) unit, ranging from 11.2% – 71% with a mean of > 22%. In contrast, the older granite (OGR) unit contains relatively less fines, ranging from 11.8% – 31% with a mean of > 17%. These findings show the significant influence of parent rock weathering on the distribution of soil fines across the lithologic units.

The liquid limit and plasticity index plotted on the Casagrande plasticity chart (Fig. 4), reveal that the tested soils predominantly lie above the A-line. According to the Unified Soil Classification System (USCS), these soils are classified as inorganic clayey silty sand (SC, SM, SC-SM) soils with low to moderately high plasticity. The soils exhibit a moderately high liquid limit, ranging from 16.5% to 53%, influenced by the high clay content (10 – 68%) observed particularly in the migmatite gneiss (MGR) and meta-sediment/volcanic (MSVR) regions. As the liquid and plastic limits are directly influenced by the type and amount of clay present in the soil, they serve as key parameters for identifying the clay fraction in soils.

The optimum moisture content (OMC) increased with decreasing maximum dry density (MDD), with OMC ranging from 8.1% - 25.0% and MDD varying from 0.9

Table 1: Descriptive statistics of 50 soil geotechnical properties

	Sand %	Silt %	Clay %	LL %	PL %	PI %	OMC %	MDD mg/m^3	CBRu %	CBRs %
	Migmatite-Gneiss region (MGR)									
Mean	65.3	20.9	30.5	30.3	16.4	13.9	14.2	1.71	7.15	3.12
Std. Dev.	9.61	9.49	13.7	9.11	7.50	4.57	4.05	0.27	5.14	1.64
Minimum	51.0	10.2	10.0	17.4	4.7	3.8	8.12	0.89	2.1	1.09
Maximum	85.0	50.8	68.0	53.0	36.9	24.4	25.0	2.61	30.4	10.6
Soil class	SC, SM, SC-SM, SP-SM									
	Older Granite region (OGR)									
Mean	54.7	17.4	24.7	24.5	14.9	9.62	13.5	1.72	18.5	9.46
Std. Dev.	9.22	5.15	5.96	6.07	3.76	4.11	2.94	0.13	6.82	2.01
Minimum	44.0	11.8	14.0	16.5	8.6	4.6	8.9	1.58	10.4	7.5
Maximum	67.0	24.2	31.0	32.4	19.0	15.3	17.0	1.91	28.4	12.3
Soil class	SC, SC-SM, GC-GM									
	Meta-sediment/meta-volcanic region (MSVR)									
Mean	62.1	22.3	35.7	36.9	20.6	15.5	15.7	1.60	7.83	3.06
Std. Dev.	9.15	9.09	15.9	6.29	5.29	4.74	3.30	0.14	3.98	1.19
Minimum	51.0	11.2	15.0	26.5	10.4	9.3	10.1	1.4	3.0	1.26
Maximum	81.0	44.3	71.0	46.5	30.7	22.6	21.1	1.86	14.7	5.54
Soil class	SC, SM, SC-SM, MH									

Note: Liquid limit (LL), plastic limit (PL), plasticity index (PI), optimum moisture content (OMC), maximum dry density (MDD), soaked and unsoaked California Bearing Ration (CBRs, CBRu), silty sand (SM), clayey sand (SC), silty clay mixture (SC-SM), poorly graded silty sand mixture (SP-SM), silt of high plasticity (MH) and gravelly silty clay mixture (GC-GM).

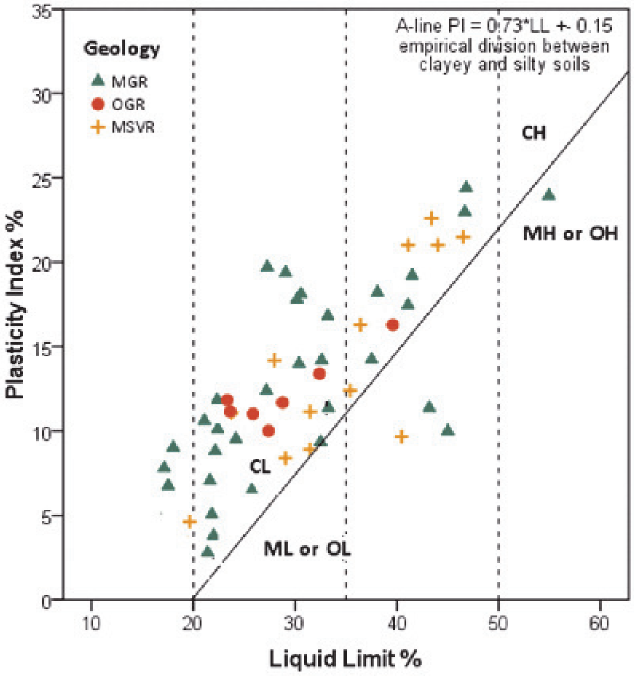

Fig. 4: Scatterplot of soil samples showing the degree of plasticity

– 2.6 mg/m^3. The highest OMC value (25.0%) was observed in the migmatite-gneiss (MGR) unit. The CBR which evaluates soil strength for road pavement design based on subgrade strength, showed partially low soaked values ranging from 1.09 – 12.3% (Table 1). These low soaked CBR values confirm the use of poor clayey lateritic soils in the subgrade and sub-base layers of the pavement. This finding underscores the inadequate suitability of the subgrade material for supporting road infrastructure, particularly in clay-rich regions.

Spectra Characteristics of Different Soil Samples

Figure 5 (a - b) presents the raw MIR spectra of soil samples, showcasing distinct absorption bands that correlate with key soil attributes. The spectra exhibit strong absorption features due to overtones and combinations of fundamental molecular vibrations. For instance, in the functional region (3800 – 3000 cm^{-1}), the signatures are related to the stretching vibrations of H-O bonds. The spectra at 3000 – 2820 and 1873 and 1730 cm^{-1} are related to C-H and C=O bonds respectively, while spectra at 1632 – 1530 cm^{-1} corresponds to the stretching and bending vibration of O-H and C-H groups. In the fingerprint region, spectra at 1409 and 1157 cm^{-1} are linked to C-H and C-O bending vibration

(Xie *et al.*, 2011). These spectral features are primariliy influenced by soil properties such as organic carbon and moisture content, which exhibit direct MIR spectral responses. As noted by Kasprzhitskii *et al.* (2018), Petit and Madejova (2013), Yavna *et al.* (2015), and Janik *et al.* (2009), significant diagnostic bands occur around 500 cm^{-1}, 1000 cm^{-1}, 3000 cm^{-1} and 3600 cm^{-1}, corresponding to stretching and bending vibrations attributable to the mineral and organic components in soils.

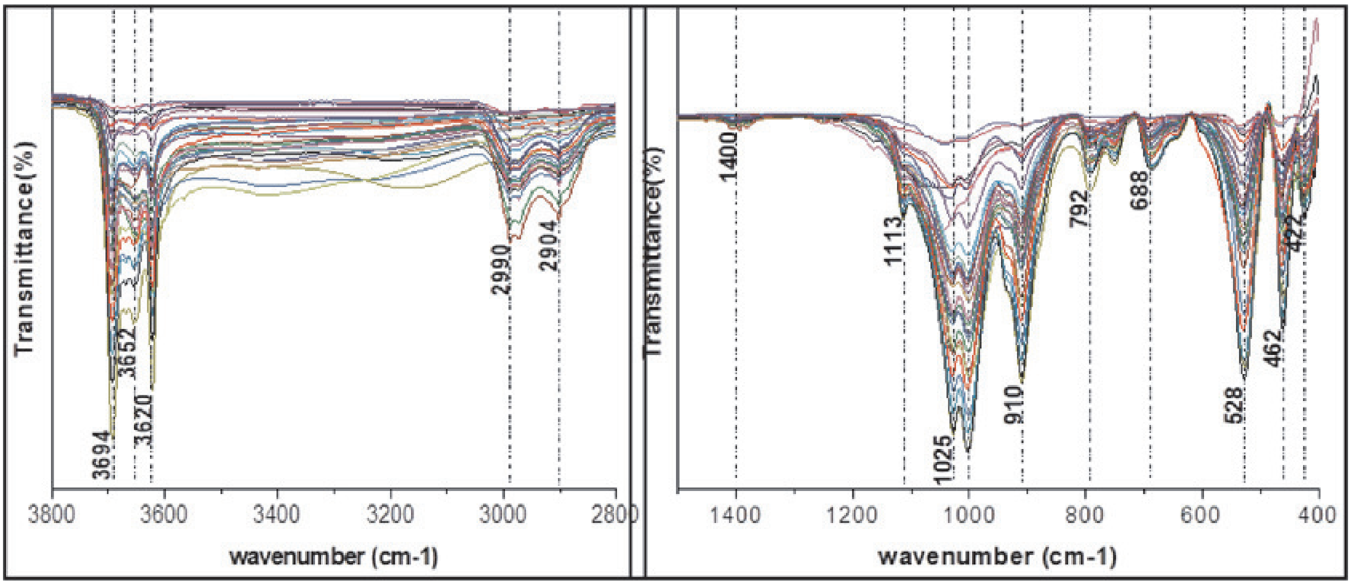

Fig. 5: Array of MIR spectra of soil samples showing strong diagnostic absorption features.

The hydroxyl (-OH) stretching and bending vibrations are prominent in the 3750 – 3300 cm^{-1} and 950 – 850 cm^{-1} regions, respectively. The Si-O stretching modes are observed in the 1150 – 950 $cm^{-1}$and 550 – 400 cm^{-1} regions, corresponding to vibrations associated with Si-O-Al and Si-O-Si bonds, characteristic of clay minerals such as kaolinite and smectite (Stenberg, 2010). The low reflectance around 3600 cm^{-1} indicates high mineral absorption of clay minerals. Additionally, distinct absorption bands at 1413 cm^{-1}, 695 cm^{-1} and 795 cm^{-1} are attributed to CO^3 stretching and CO^3 deformation, suggesting the presence of calcite in the soil samples.

Performance of Partial Least Square Regression

Accurate prediction models were developed using MIR spectra for six soil properties: sand, clay, liquid limit (LL), plastic limit (PL), plasticity index (PI), and soaked California Bearing Ratio (CBRs). These models achieved R^2 and RPD values greater than 0.7 and 2, respectively, indicating robust predictive performance (Table 2). Figure 6 presents scatterplots comparing MIR-predicted and laboratory-measured values for the validation set, along with a 1:1 reference line. The prediction of sand and clay content are consistent with prior studies that reported R^2 values of 0.8 – 0.96 for these parameters (e.g. Wartini *et al.*, 2022; Madari *et al.*, 2006; Selige *et al.*, 2006). These accuracies are attributed to the fundamental vibrations associated with clay minerals (e.g., kaolinite: 3690-3620 cm^{-1}, smectite: 3630-3620 cm^{-1}, illite: 3400-3300 cm^{-1}, and quartz: 1100-1000 cm^{-1}) (Soriano-Disla *et al.*, 2014). However, models for silt content, optimum moisture content (OMC), maximum dry density (MDD), and unsoaked CBR (CBRu) yielded poor predictions (RPD < 1.4) and were excluded from the analysis. For the Atterberg limits, the predictions for LL, PL, and PI achieved R^2> 0.7, aligning with previous studies (e.g., Yitagesu *et al.*, 2009; Waruru *et al.*, 2014; Mousavi *et al.*, 2019), which reported similar high coefficients. The regression models were derived from the first three principal components (PC1, PC2, PC3), which collectively explained over 90% of the variance in MIR spectra (Table 2). These findings underscore the capability of MIR spectroscopy in predicting soil index properties, which are critical parameters in engineering studies.

Conclusion

Investigation of large-scale soil properties still remains a significant challenge that need be surmounted in a cost-effective manner owing to high cost, labour

Table 2: Prediction model performance indicators for PLSR

SOIL VARIABLES	MSE	RMSE	R^2	RPD	PC1	PC2	PC3	Intercept
Sand %	2.7	1.64	0.77	3.18	0.01	-0.14	-0.08	63.2
Clay %	1.63	1.28	0.86	4.25	-0.05	0.136	0.067	27.3
LL %	2.36	1.78	0.72	2.46	-0.07	-0.03	0.174	30.3
PL %	2.13	1.46	0.76	3.14	-0.06	0.134	0.11	19.4
PI %	0.99	1.21	0.78	3.64	-0.01	-0.16	0.064	10.9
CBRs %	2.05	1.75	0.72	2.51	0.01	-0.01	-0.08	16.5

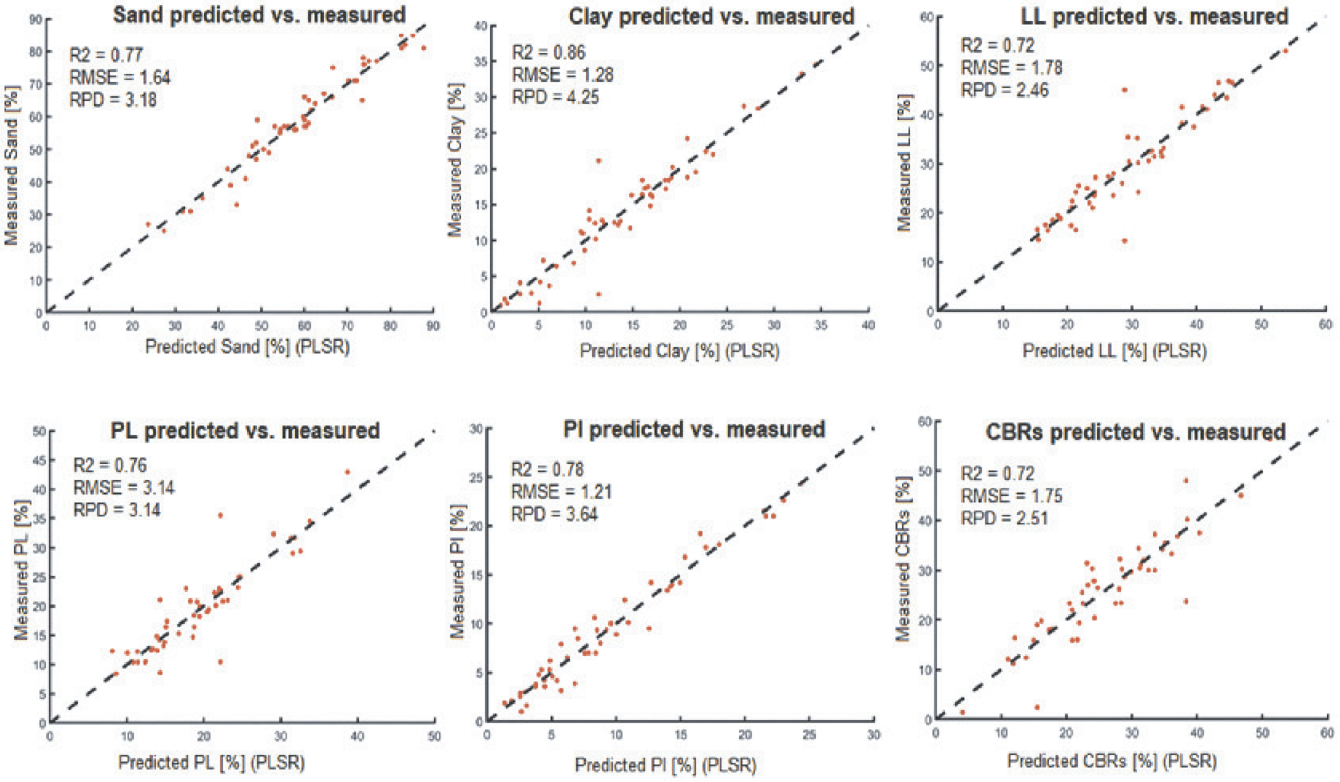

Fig. 6: Scatter plots of laboratory-measured versus MIR-predicted soil properties using PLSR

intensive and time-consuming analysis. This study demonstrated the efficacy of mid-infrared (MIR) spectroscopy as a simple, non-destructive, and rapid technique for estimating key soil engineering properties using partial least square regression (PLSR). The results highlighted that six soil properties - sand, clay, LL, PL, PI and CBRs were modeled with robust quality indices (RMSE < 1.8, R^2> 0.72, RPD > 2.5). The strong predictive performance for plasticity and texture was attributed to the strong correlation between these properties and spectrally active components, particularly clay mineralogy (e.g., O-H bonds and Fe oxides). The high correlation and performance (R > 0.7) observed in soil texture, plasticity, and CBR prediction underscore the potential of MIR spectroscopy in complementing traditional soil analysis methods. This study provides new insights into the application of MIR technology for estimating soil properties effectively. Therefore, we recommend the use of MIR spectroscopy as a complementary approach to conventional methods for soil property estimation due to its rapid, cost-effective, and reliable performance.

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