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Spectral soil analysis for fertilizer recommendations by coupling with QUEFTS for maize in East Africa: A sensitivity analysis

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ABSTRACT

Laboratory analysis of soil properties is prohibitively expensive and difficult to scale across the soils in sub-Saharan Africa. This results in a lack of soil-specific fertilizer recommendations, where recommendation can only be provided at a regional scale. This study aims to assess the feasibility of using spectral soil analysis to provide soil-specific fertilizer recommendations.

Using a range of spectrometers [NeoSpectra Saucer (NIR), FieldSpec 4 (vis-NIR) with contact probe or mug light interface, FTIR Bruker Tensor 27 (MIR)], 346 archived soil samples (0–20 cm) with known soil chemical properties collected from Ethiopia, Kenya and Tanzania were scanned. Partial least square regression (PLSR) was used to develop prediction models for selected soil properties including pH, soil organic carbon (SOC), total nitrogen, Olsen P, and exchangeable K. These predicted properties, and associated uncertainty, were used to derive fertilizer recommendations for maize using the Quantitative Evaluation of the Fertility of Tropical Soils (QUEFTS) model parameters for sub-Saharan Africa.

Most soil properties (pH, SOC, total nitrogen, and exchangeable K) were well predicted (Concordance Correlation Coefficient values between 0.88 and 0.96 and Ratio of Performance to Interquartile values between 1.4 and 5.9) by all the spectrometers but there were performance variations between soil properties and spectrometers. Use of the predicted soil data for the development of fertilizer recommendations gave promising results when compared to the recommendations obtained with the conventional soil analysis. For example, the least performing NeoSpectra Saucer over/under-estimated up to 8 and 24 kg ha^{-1}N and P, respectively, though there was insignificant variation in estimation of P fertilizer among spectrometers. We conclude that spectral technology can be used to determine major soil properties with satisfactory precision, sufficient for specific fertilizer decision making in East Africa, possibly even with portable equipment in the field.

1. Introduction

Intensified farming with increased productivity is necessary in many regions of the world to match the growing food and energy demand. Among many management factors, mineral fertilizer use is regarded as an essential component in agricultural intensification. Fertilizers play a key role in providing global food supplies and will continue to be needed even with climate change (Wortmann and Sones, 2017; Krasilnikov et al., 2022). To optimize their use, soil tests can help to identify whether it would be productive to grow a particular crop in an area, what fertilizer to apply and how much of it. However, an important constraint in the judicious use of fertilizers in Africa arises from inadequate, often slow and expensive soil testing facilities with limited capacities (Shepherd and Walsh, 2002). Historically, soil laboratories have been under-supported in many developing countries resulting in poor quality diagnosis, which quickly leads to inappropriate fertilizer recommendations, reduced productivity and higher costs.

Furthermore, conventional soil analysis methods not sufficiently standardized between different laboratories hamper attempts to compare and synthesize soil measurements from different countries,

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regions, times, and studies making it difficult to reliably extrapolate findings. A resulting practice is the use of blanket fertilizer recommendations for whole regions, often causing the continuous use of imbalanced fertilizer rates and low nutrient use efficiency (Tittonell et al., 2008; Ichami et al., 2019). This is not adequate because the soil environment is dynamic, varying tremendously across space and time, and thereby affecting the resource use efficiency in many agricultural systems (Tittonell et al., 2008). The development of cost-effective soil analysis methods is becoming a priority in contemporary soil science (Grunwald et al., 2011), and this is particularly important when considering the creation of new, harmonized, target-scale spatial soil datasets.

The trade-off between the growing need for large scale soil information and its high cost could be resolved by a widespread use of diffuse reflectance soil spectroscopy (DRSS) in the visible-near infrared (vis-NIR) and the mid infrared (MIR) regions. The diffusely reflected/absorbed spectral signatures have been proven to reliably predict important soil properties (Viscarra Rossel et al., 2016; Lausch et al., 2013; Bah et al., 2016; Shepherd & Walsh, 2007). They were also applied in digital soil mapping (Paul et al., 2019; Morais et al., 2018; Hengl et al., 2021; Brodský et al., 2011), evaluated for crop productivity and performance estimation (Breure et al., 2021), and for fertilizer decision making using a soil fertility categorical approach (Ng et al., 2020). Therefore, these tools could be useful to improve fertilizer decision making in low-income countries for higher agricultural productivity through informed decisions which can be continuously improved and updated.

One of the advancements in soil spectroscopy is the development of diverse spectrometers which can be suitable for various applications with a range of costs, precision, and flexibility while in use. The soil scanning spectrometers employed in soil science are mostly operating in the vis-NIR (350–2500 nm), NIR (1350 – 2500 nm) or MIR (2500–16700 nm) spectrum with diverse equipment setups such as bench-top, portable or handheld spectrometers. These spectrometers further differ in their technical specifications which encompasses the type of light source and detector, measurement principles, energy intensity and resolution (Mouazen et al., 2007; Dos Santos et al., 2013; Rodionov et al., 2016; Xu et al., 2016; Fajardo et al., 2017; Ng et al., 2019). These differences may result in varied precision and consistency across soil properties, soil types and scanning conditions. The spectrometers also differ in weight, size, and sample preparation protocols (Tang et al., 2019) which may affect the speed of analysis, sample processing duration, cost of soil analysis and ability to perform measurements in the field. Particularly, the MIR spectroscopy provides clear and distinct absorbance peaks, however, the technology is more complex, demands better facilities and training and often liquid nitrogen to cool down the light source which may not be accessible easily in developing countries. It is also more costly compared with vis-NIR and NIR spectroscopy (Li et al., 2022; Reeves, 2010; Viscarra Rossel et al., 2006). In contrast, vis-NIR and NIR spectroscopy are robust methods that do not require much soil preparation (Sharififar, 2019) and can be integrated into simpler scanning instrumentations for reduction in cost and field applicability.

A number of studies have compared and evaluated various soil scanning instrumentations and spectral ranges for their precision, consistency, cost and complexity in obtaining spectral recordings (Van Groenigen et al., 2003; Mouazen et al., 2005; Bellon-Maurel & McBratney, 2011; Ge et al., 2011; Xie et al., 2011; Soriano-Disla et al., 2014; Piikki et al., 2016; Gates, 2018; Hutengs et al., 2018; Pätzold et al., 2020; Sharififar, 2019; Tang et al., 2019). However, most comparisons of soil scanning instrumentations were carried out on a small number of soil properties, particularly soil organic carbon (SOC) and clay content (Knadel et al., 2013); soil moisture content and some chemical properties of manures (Mouazen et al., 2005); and SOC and total carbon estimation (Sharififar, 2019). Further comparisons on the predictive accuracy and instrument-specific trade-offs are needed to understand relationships among the scanning outcomes and prediction performance for a specific soil property (Knadel et al., 2013; Cécillon et al., 2009; Breure et al., 2022; Clingensmith et al., 2019).

Furthermore, the soil information generated should be interpreted in relation to its use, in our case fertilizer recommendations. Among other approaches to interpret the soil information, mechanistic or empirical soil-crop-fertilizer models such as the QUEFTS model (**QU**antitative **E**valuation of the **F**ertility of **T**ropical **S**oils) and soil test-based (STB) fertilizer recommendation models have been used to determine the amount of nutrients to be applied (Janssen et al., 1990; Tittonell et al., 2008; Sattari et al., 2014).

But it remains unclear if cheaper spectrometers can provide sufficient prediction accuracy to provide meaningful fertilizer recommendations (Tang et al., 2019; Sharififar, 2019). Hence, this study aims to i) compare the performance of desktop and portable soil scanning infrared instruments with conventional reference soil analysis techniques and in predicting multiple soil properties and ii) to use these predictions to derive and evaluate fertilizer recommendations for maize grown in selected soils of East Africa.

2. Materials and methods

2.1. Soil sample sources

The soil samples used in this study were archived at the Africa Soil Information Service (AfSIS) spectral laboratory of Rothamsted Research, UK. They have been collected from Ethiopia, Kenya and Tanzania during different research projects viz., the Geo-Nutrition project (BB/P023126/1) in Ethiopia, the iCGRAF project (also BB/P023126/1) in Kenya and Tanzania, and a second Geo-Nutrition project funded by the Bill and Melinda Gates Foundation (INV-009129). A total of 346 topsoil (i.e., 0–20 cm depth) samples were used for this study, representing a wide-ranging agroecology and many soil types. Geographically, there were 15, 259 and 76 soil samples from Ethiopia, Kenya and Tanzania, respectively. Samples were air dried, crushed with a pestle and mortar and sieved to pass through a 2 mm stainless steel sieve. Then, subsamples were further fine milled (<50 μm) and stored in glass vials with a screw cap for scanning.

2.2. Soil spectral data collection with a brief description of spectrometers

The soil samples were scanned using four different commercially available spectrometers (Fig. 1) whose characteristics are summarized in Table 1. Technical descriptions of each infrared spectrometers are briefly presented below including the labelling used in brackets for each spectrometer in the graphs and discussions afterwards.

- *FTIR Bruker Tensor 27 bench-top spectrometer (Tensor-II) (Fig. 1 a) was used to collect the spectral data in the MIR region (FTIR Bruker Tensor 27; Bruker Optik GmbH, Ettlingen, Germany) using a nitrogen purged integrating sphere to cool the MCT (mercury cadmium telluride) mid-band detector. The high throughput screening accessory (HTS-XT), which scans 95 samples in one plate, was used with a spectral resolution of 4 cm^{-1} and scan time of 32 s per sample. Absorbance data in the spectral range 2500–16,666 nm were obtained in two replicates.*
- *The portable ASD Contact Probe (FS4-CP) (Fig. 1 b) together with the FieldSpec 4 (2019 Malvern Panalytical) spectrometer, is used to measure samples through contact which minimizes measurement errors associated with stray light. The light source for this spectrometer is a Halogen bulb/1500 h with a colour temperature of 2900 k that requires 12–18 VDC and 6.5 W. It had a 3 nm vis, 8 nm short-wave infrared (SWIR) spectral resolution with wavelength accuracy of 0.5 nm. Three repeated scans were taken in the same sample holder/Petri dish by moving the 12 mm diameter visNIR sensor each time.*
- *The portable ASD Mug light (FS4-ML) (Fig. 1 c) together with the FieldSpec 4 (2019 Malvern Panalytical) spectrometer, is employed to*

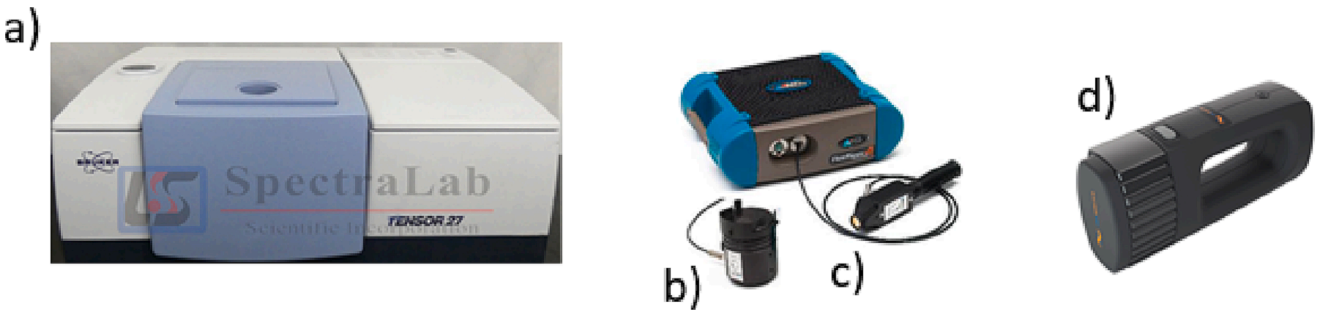


Fig. 1. Spectrometers compared in this study: a) FTIR Bruker Tensor 27 (Tensor-II), b) FieldSpec 4 mug light (FS4-ML) and contact probe (FS4-CP); and c) NeoSpectra Saucer (Neospec).

Table 1
Characteristics of the spectrometers compared [FTIR Bruker Tensor 27 (Tensor-II), FieldSpec 4 mug light (FS4-ML) and contact probe (FS4-CP), and NeoSpectra Saucer (Neospec)].

Spectrometers	Spectral region (nm)	Spot size (mm)	Unit price (£) *	Weight (kg)	Power source	Spectra data points
Tensor-II	MIR/NIR 1340–16669	6	71,163.00	>30.0	DC	2376
FS4-CP	Vis-NIR 350–2500	10	75,140.00	6.1	AC	2151
FS4-ML	Vis-NIR 350–2500	12	72,950.00	6.7	AC	2151
Neospec	NIR 1339–2500	10	3,850.00	1.0	AC	1023

*Prices were collected in July 2021.

acquire reflectance and absorbance measurements of samples using the ASD sampling tray adapter. This scanning interface has the advantage of minimizing measurement errors related to stray light and specular reflected components. The light source for this scanning interface is a Tungsten Quartz Halogen b/1500hrs with a bulb colour temperature of 2900 k. It had a 3 nm vis, 8 nm short-wave infrared (SWIR) spectral resolution with wavelength accuracy of 0.5 nm. Three replicate measurements of each soil sample were acquired with independent subsamples placed on the ASD sampling tray adapter.

- *NeoSpectra Saucer (Neospec) spectrometer (Fig. 1 d) is a hand-held Near InfraRed (NIR) spectral sensor manufactured by Si-ware containing a single-chip Michelson interferometer with monolithic opto-electro-mechanical (OEM) structure (Si-ware, 2017). It has a wavelength resolution of 16 nm and a wavelength accuracy of ± 1.5 nm. The sample scanning was performed with the settings set to boxcar, 3 N zero padding and a 10 s integration resulting in 1024 data points per spectrum using linear interpolation. Three replicate measurements per sample were recorded by moving the scanning spot over the soil sample in a petri dish.*

2.3. Conventional soil analysis

The dry combustion method was used to determine total carbon (Nelson and Sommers, 1996) and total nitrogen (Bremner, 1996) with a Leco dry combustion analyzer (Stockport, UK). Inorganic carbon was analyzed using wet acidification with a Skalar Primacs AIC 100 (Skalar Analytical BV, Breda, Netherlands). Soil total organic carbon (SOC) was then calculated by subtracting inorganic carbon from total soil carbon. The Cobalthexamine extract (ISO 23470) of exchangeable K was analyzed with inductively coupled plasma optical emission spectrometry (ICP-OES) (Ciesielski and Sterckeman, 1997). Soil pH was measured in a 1:2.5 soil: water suspension (ISO 10390: 2005) one hour after mixing, using a thin semi-micro sealed combined pH electrode from Fisher scientific (Loughborough, UK). Olsen P was measured in the sodium bicarbonate extract (Olsen, 1954) using the phospho-molybdenum blue method on a continuous colorimetric flow analyzer.

2.4. Soil property prediction from spectra

2.4.1. Spectral pre-processing

The MIR scans of the Tensor II were converted to wavelengths (nm). The reflectance (R) measurements recoded by all spectrometers were transformed to the logarithmic apparent absorbance using $A = \log(1/R)$. Splice correction (de-stepping) on FS4-ML and FS4-CP at 1000 and 1800 nm was performed using the "spliceCorrection" function in the "prospectr" package (Stevens and Lopez, 2014) in R (R Core Team, 2017). The spectral records of FS4-ML and FS4-CP outside the 500–2450 nm range and of Neospec beyond 2450 nm were removed because of the low signal-to-noise ratio often caused by light scattering effects of quartz sand or by instrument drift. This was followed by performing a combination of spectral pre-processing techniques that improved absorption features by reducing the noise (the Savitzky-Golay Smoothing with spectral first derivative) (Vestergaard et al., 2021). The smoothing gap sizes were a window of 11 nm for vis-NIR and MIR and a window of 5 nm for NIR. Thereafter, the spectral data was cleaned from water absorption regions (H_2O band 1 between 1350 and 1460 nm; H_2O band 2 between 1790 and 1960 nm) in the vis-NIR, and CO_2 peaks in the MIR absorption regions (between 4274 and 4464 nm).

2.4.2. Principal component analysis and

A principal component (PC) analysis was performed to generate the PC scores of the respective infrared regions recorded from each spectrometer that explained 99 % of the variation using the "resemble" R package (Ramirez-lopez et al., 2022).

2.4.3. sub-dividing samples into train and test sets

The dataset was split into a calibration (training) set (75 %) and independent test set (25 %) using the conditioned Latin Hypercube sampling in the spectra PC score space. Thus, after removing the outliers (Supplementary Material Fig. 1), 260 and 86 samples were used, respectively. Supplementary Fig. 2 shows the spread of the training and the independent test sets in the score plot of the first two PCs for each spectrometer.

2.4.4. Model calibration and performance evaluation

Partial least squares regression (PLSR) was used to develop predictive models of each soil property from the calibration spectra using the "pls" package (Wehrens, 2007). The number of components to retain were chosen based on the minimum root-mean squared error estimated from a tenfold cross validation. Models for each spectrometer were then evaluated on the independent test set. The performance of predictive

models was evaluated using concordance correlation coefficients (CCC), the Ratio of Performance to Inter Quartile distance (RPIQ), the Root Mean Square Error (RMSE) and the Bias, quantified using the independent test set. CCC measures both the accuracy and precision (Lin, 1989) with a range of values between − 1 and + 1, where a value of + 1 denotes a perfect agreement.

2.5. Derivation of soil test-based fertilizer estimation

2.5.1. Estimation of indigenous soil nutrient supply (NPK)

Based on the Quantitative Evaluation of the Fertility of Tropical Soils (QUEFTS) model, the indigenous soil supply of N, P and K were derived from the empirical relationship of values of SOC, Olsen P and exchangeable K with pH and SOC according to Eqs. [1–3], respectively (Janssen et al., 1990; Tittonell et al., 2008; Sattari et al., 2014).

$$SNj = fNj \times 6.8 \times SOCj \tag{1}$$

$$SPj = fPj \times 0.35 \times SOCj + 0.5 \times Olsen\,Pj \tag{2}$$

$$SKj = \frac{fKj \times 500 \times Exchangeable\,Kj}{2 + (0.9 \times SOCj)} \tag{3}$$

where SN, SP and SK are the indigenous soil supply of N, P and K, respectively, from soil mineralization and expressed in kg ha^{-1}; SOC is organic carbon content of the soil expressed in g kg^{-1} of soil; P and K are expressed in mg kg^{-1} and cmol kg^{-1} soil, respectively; and j is the soil testing (conventional as well as spectral soil analysis) methods. Soil pH correction factors were used according to Eqs. [4–6] because pH considerably influences N mineralization, P dissolution and K exchangeability from soils (Sattari et al., 2014).

$$fNj = f(x) = \begin{cases} 0.4, pH_j < 4.7 \\ 0.25 \times (pH_j - 3), 4.7 < pH_j < 7 \\ 1, pH_j > 7 \end{cases} \tag{4}$$

$$fPj = f(x) = \begin{cases} 0.02, pH_j < 4.7 \\ 1 - 0.5 \times (pH_j - 6)^2, 4.7 < pH_j < 6 \\ 1, 6 < pH_j < 6.7 \\ 1 - 0.25 \times (pH_j - 6.7)^2, 6.7 < pH_j < 8 \\ 0.57, pH_j > 8 \end{cases} \tag{5}$$

$$fKj = f(x) = \begin{cases} 1, pH_j < 4.5 \\ 6.1 \times (pH_j)^{-1.2}, 4.5 < pH_j < 6.8 \\ 0.6, pH_j > 6.8 \end{cases} \tag{6}$$

where fN, fP, and fK are pH-H_2O correction factors for N, P and K, respectively, and j is the soil testing method.

2.5.2. Estimation of nutrient requirement for maize

We estimated fertilizer recommendations based on Rurinda et al. (2020), [Eq. (7)] for the Sub-Saharan region in this study. In addition, some key assumptions were considered for estimating the nutrient requirements of maize. These include, firstly, the maize target yield is 7 t ha^{-1}, which is a median of the yield range from 6 − 13 t ha^{-1} retrieved from the Global Yield Gap Atlas protocol (i.e., www. yieldgap.org) for the East Africa region, assuming that the attainable yield is 70 % of the water limited yield potential. Secondly, we assumed that the optimum requirement of each nutrient in kg per tonne of maize grain is between the inverse of the maximum accumulation and dilution of the crop specific internal efficiencies (Smaling and Janssen, 1993). Hence, we took the average of the inverse internal efficiencies reported by Rurinda et al. (2020) for East Africa for each nutrient (for N ~ 16.74; for P ~ 3.02; and for K ~ 15.44). Thirdly, the fertilizer recovery efficiency used in this study for N and K was 50 % as reported by Sattari et al. (2014), and 30 % for P as reported by Rurinda et al. (2020). Thus, the NPK requirements are calculated according to:

$$NC_{ij} = \frac{(NR_i \text{ x } Y_{at}) - (S_{ij})}{RE_i} \tag{7}$$

where NC is the crop nutrient input requirement in kg ha^{-1}; NR is the N, P or K kg requirement per tonne of maize grain; Y_{at} is the attainable maize grain yield target in t ha^{-1}; S is the indigenous nutrient supply of N, P or K derived from equation 2–4; and RE is the recovery efficiency for applied nutrients (%, ratio of crop nutrient uptake to nutrients applied); $_i$ is N, P or K; $_j$ is the soil testing method.

2.6. Bootstrapping and error propagation

Our calibration set was selected with a model-based sampling strategy and is, thus, controlled by design (Wehrens et al., 2002). Hence, we used the non-parametric bootstrapping (10,000 iterations) by residuals method to estimate the uncertainty of PLS predictions (Zhang, 2014) by deriving the leverage and residuals of the calibration set which is outlined in the Supplementary Material [Eqs. 1–2]. Then, the confidence intervals were estimated by the bias-corrected method. Firstly, the bias was estimated as the proportion of individual bootstrap estimates that exceed the overall bootstrap mean (p_b). The proportional bias was then converted to standard normal deviates using the inverse (quantile) normal distribution function ($b = \Phi^{-1}(p_b)$). Twice that bias was then subtracted from the standard normal 95 % confidence interval limits (z) which were converted to proportions by use of the normal (probability) distribution function. The percentiles were thus given by [Eqs. 10–11]:

$$\alpha_1 = \Phi\left(b + \frac{b + z^{(\alpha/2)}}{1 - b + z^{(\alpha/2)}}\right) \tag{10}$$

$$\alpha_2 = \Phi\left(b + \frac{b + z^{(1-\alpha/2)}}{1 - b + z^{(1-\alpha/2)}}\right) \tag{11}$$

where, $z^{(\alpha/2)}$ was the $100 \times \left(\frac{\alpha}{2}\right)^{th}$ percentile point of the normal (probability) distribution function (e.g., $z^{(05/2)} = -1.96$). The standard deviation of each individual prediction was then computed as the difference between the confidence limits divided by twice the 95 % normal deviate: $\sigma = \frac{CI_u - CI_l}{2z}$, where: $2z = 3.92$.

The standard deviations associated with predictions for the validation set were used to propagate marginal prediction errors in the estimation of indigenous soil N and K supply (Supplementary Material [Eqs. 3–5]). Finally, uncertainty in the indigenous soil N and K supply was propagated into the nutrient requirement for a given yield target (Eq. (7)) from the soil nutrient supply of N and K as follows:

$$\sigma_{N_{ij}} = \sqrt{\left(\frac{\sigma^2_{S_{ij}}}{S^2_{ij}}\right)} NC_{ij} \tag{12}$$

Given that Olsen P was log-transformed for the PLS regression, we propagated the 100(1-α/2)% confidence interval (CI) limits through in the equations for the soil P supply (Eq. (2)), correction factor (Eq. (5)), and P requirement (Eq. 7) for CI_l, the mean over all the bootstrap estimates and CI_u of pH, SOC and Olsen P. Thus, the uncertainty in SOC predictions was disregarded for error propagation in the P requirement.

3. Results

3.1. Description of the soil properties

Table 2 presents descriptive statistics of the soil properties obtained by conventional analysis separately for the calibration and independent test sets. Soil pH ranged from 4.37 to 8.89 well representing the diverse pH values in agricultural soils of the region. The average, as measured by the mean (for most properties) or median (for the skewed Olsen P), of the soil attributes for all properties, were comparable in the calibration and independent test sets. Olsen P data was highly skewed, and a log

Table 2
Descriptive statistics of soil chemical properties for model training and independent test set.

Soil property	Sample set	N	min	q1	median	mean	q3	max
pH	Cal	260	4.48	5.09	5.50	5.99	6.42	8.89
	val	86	4.37	5.06	5.48	5.96	6.37	8.76
SOC	Cal	260	0.50	1.12	1.42	1.42	1.67	2.45
	val	86	0.57	1.15	1.40	1.43	1.70	2.51
TotalN	Cal	260	0.04	0.09	0.11	0.11	0.13	0.20
	val	86	0.04	0.09	0.11	0.11	0.13	0.20
Exch.K	Cal	260	1.02	2.28	3.81	6.69	7.81	45.83
	val	86	0.57	2.62	3.55	6.35	8.54	36.87
OlsenP	Cal	260	0.42	3.53	6.41	10.17	11.30	89.96
	val	86	0.94	3.98	6.40	8.99	10.87	35.62

transformation was carried out before calibrating the predictive models from the spectra based on an investigation of the PLSR residuals for model calibration and back-transformed for the prediction exercise. Supplementary Table 1 further separates these statistics by country.

3.2. Soil property prediction accuracy and consistency for QUESFTS inputs

The prediction performance with the associated prediction error for the independent test set of all spectrometers is depicted in Fig. 2. As shown in this figure, all soil properties except Olsen P were adequately predicted from spectra obtained from all spectrometers, as indicated by CCC values ranging from 0.77 to 0.96 and RPIQ values between 1.7 and 4.7. In particular, soil pH was predicted with higher precision and consistency, when compared to other soil properties considered, by the vis-NIR, NIR and the MIR spectrometers. Furthermore, SOC, exchangeable K and total N were slightly better predicted by the vis-NIR and MIR spectrometer than the NIR spectrometer. Predictions from NIR spectrometer resulted in the lowest RPIQ values for SOC, exchangeable K and total N (2.1, 1.7 and 2.2, respectively) though the values are still in the range of model stability and reproducibility. The CCC and RPIQ values for vis-NIR and MIR spectrometers are in the category of good model performance and consistency whereas the respective values for NIR would be categorized as moderate according to Viscarra Rossel et al. (2016). This could have arisen from the missing absorbance ranges between 500 and 1350 which are clearly informative as demonstrated in the loadings plots shown in Supplementary Material Fig. 3 - Fig. 7. Across all four spectrometers, the spectra generated from the MIR spectrometer excelled in predicting SOC and total N, showing higher precision and consistency than any of the other spectrometers.

Across soil properties, Olsen P had the poorest agreement with larger errors than all other soil properties. This indicated that Olsen P prediction using the spectroscopic analysis was more uncertain than for the other soil properties considered. As can be seen from the scatter plot (Fig. 2), the deviation between the predicted and measured Olsen P increased above 15 mg P kg^{-1} irrespective of the spectrometer. Overall, there was a tendency to underestimate higher values of Olsen P (>15 mg P kg^{-1}) and exchangeable K (>25 cmol kg^{-1} soil) by all soil

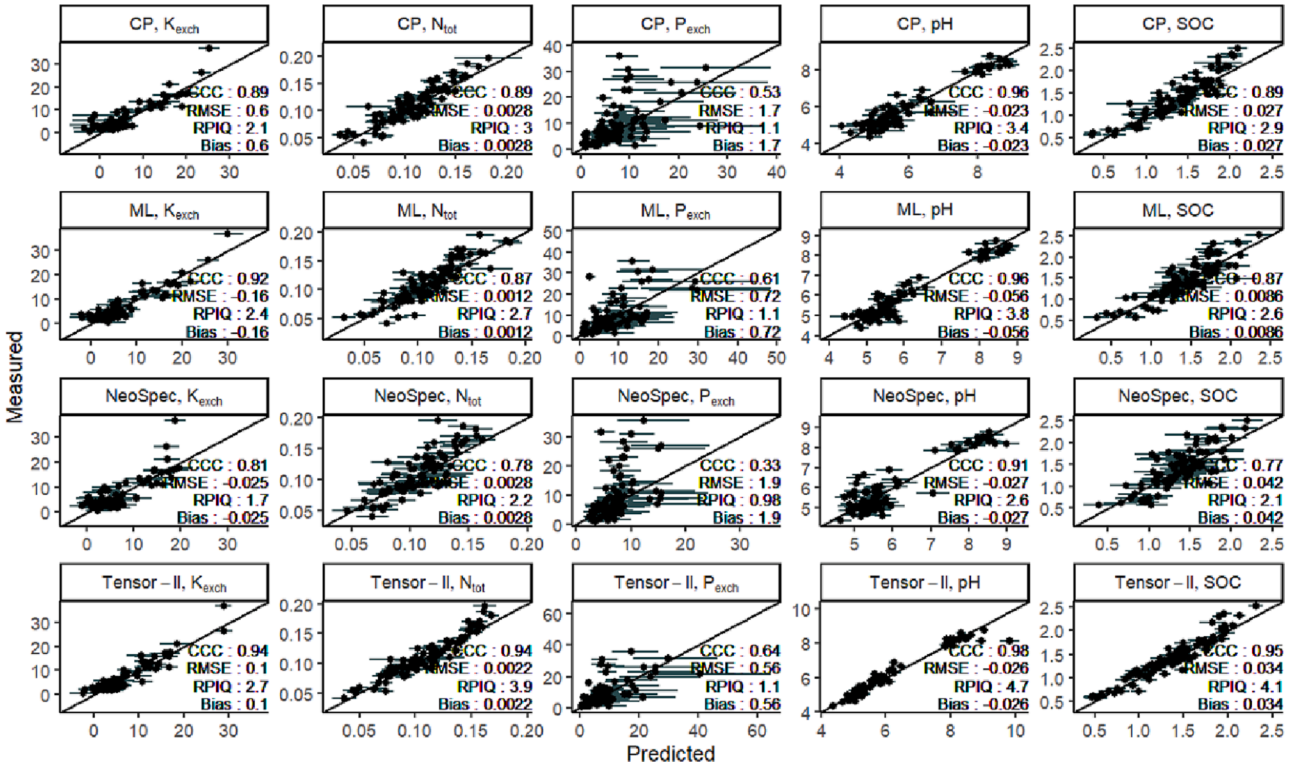


Fig. 2. Prediction accuracy and consistency for all soil properties (exchangeable K, total N, Olsen P, pH, and SOC, respectively) and spectrometers (FS4-CP -> FieldSpec 4 contact probe, FS4-ML -> FieldSpec 4 mug light, Neospec -> NeoSpectra Saucer, Tensor-II -> FTIR Bruker Tensor 27). The statistics shown are the root mean square error (RMSE), the concordance correlation coefficient (CCC), Bias and the ratio of performance to interquartile range (RPIQ). The horizontal lines are the error bars which represented 95 % confidence intervals.

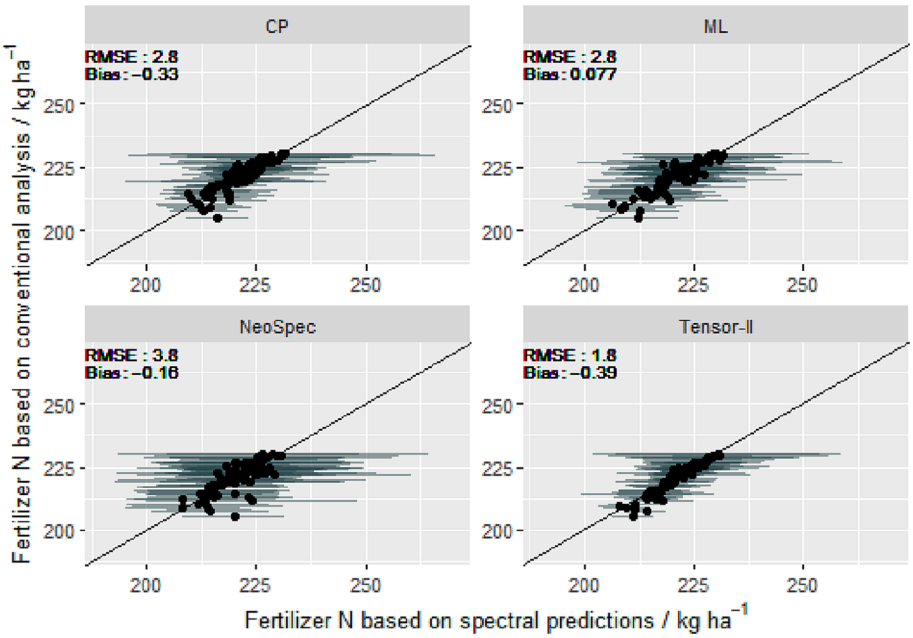


Fig. 3. *Nitrogen fertilizer rate predictions for a 7 t ha^{-1} target maize yield based on spectral (x-axis) and conventional (y axis) soil analysis. The statistics shown are the root mean square error (RMSE) and Bias for each spectrometer (FS4-CP -> FieldSpec 4 contact probe, FS4-ML -> FieldSpec 4 mug light, Neospec -> NeoSpectra Saucer, Tensor-II -> FTIR Bruker Tensor 27). The horizontal lines are the marginal uncertainties represented as ± 1σ.*

spectrometers.

3.3. Comparison of soil testing methods for fertilizer decision making

There was no potassium fertilizer recommended for a 7 t ha^{-1} maize grain yield target because all studied soil samples had sufficient plant available K supply (Table 2). Hence, we only included nitrogen and phosphorus recommendation results.

3.3.1. Nitrogen fertilizer recommendation

Fig. 3 shows the scatter plot of the estimated nitrogen requirements using the spectra from the spectrometers versus the conventional soil analysis methods for a 7 t ha^{-1} yield target with a 95 % confidence interval (CI). The MIR spectrometer had the lowest RMSE (1.8 kg ha^{-1}) for recommended nitrogen fertilizer rates while the RMSE were 2.8, 2.8 and 3.8 kg ha^{-1} for the vis-NIR contact probe sample interface, the mug light sample interface and the NIR, respectively. However, the vis-NIR FS4

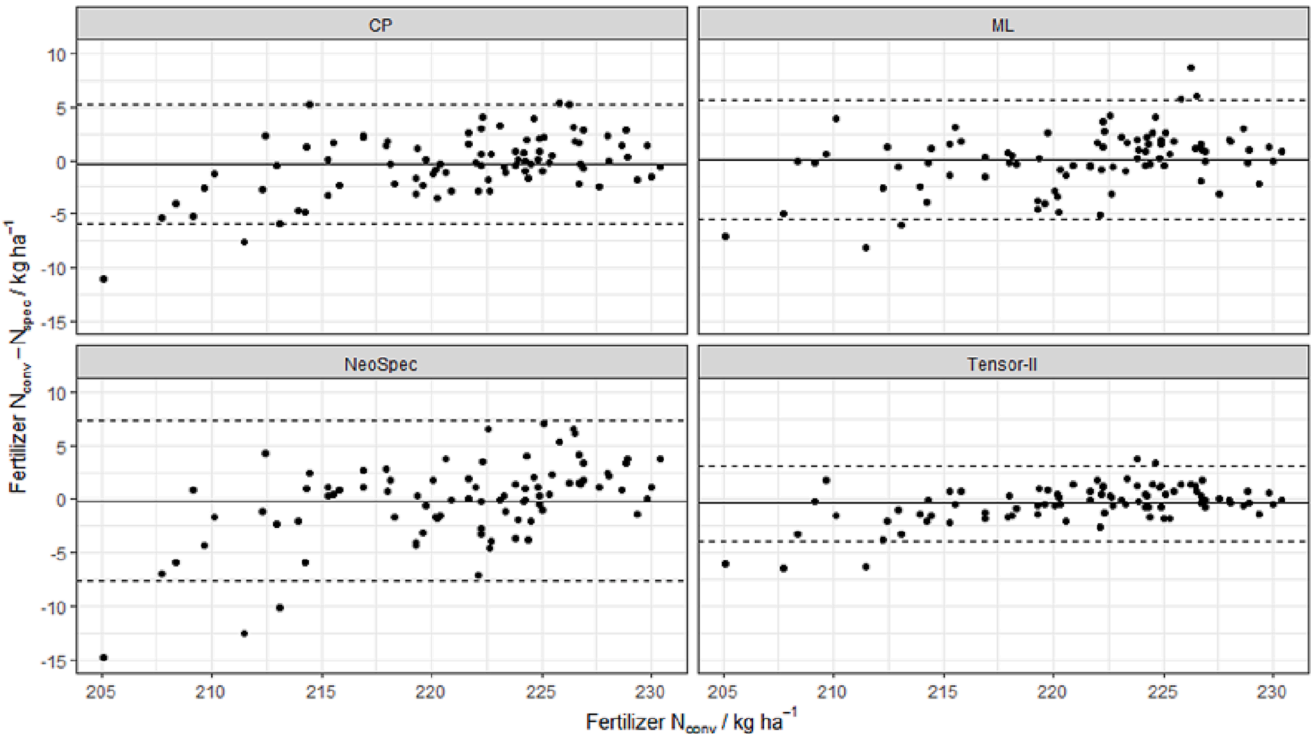


Fig. 4. Fertilizer N difference among the conventional and spectrometers (FS4-CP -> FieldSpec 4 contact probe, FS4-ML -> FieldSpec 4 mug light, Neospec -> NeoSpectra Saucer, Tensor-II -> FTIR Bruker Tensor 27). The dashed horizontal lines are the mean difference $\pm z^{(\alpha/2)}\sigma$ and the horizontal line is the mean difference.

contact probe and MIR spectrometer resulted in a higher bias than the other two spectrometers. The recommended nitrogen fertilizer rates from all spectrometers were comparably close to each other and fell close to the 1:1 line with the fertilizer rate determined based on conventional soil analysis.

There was a tendency for wider confidence intervals at higher rates of estimated nitrogen fertilizer from predictions based on the contact probe spectrometer and in particular for the Tensor II (Fig. 3; Fig. 4) while the confidence intervals are consistent for the other two spectrometers. Between spectrometers, the confidence intervals and the distance between the lower and upper bounds of the 95 % fertilizer N estimation difference between the spectrometers and conventional method were narrower with MIR followed by vis-NIR and then NIR, confirming a better performance of the former than the rest of the spectrometers (Fig. 4). The NIR predictions resulted in the widest confidence interval and 95 % fertilizer N estimation difference (-7.61 to 7.29 kg N ha^{-1}), however the difference was not prominent. Meanwhile the 95 % fertilizer N estimation differences lied in a range of −3.86 to 3.07, 5.43 to 5.59, and −5.84 to 5.17 kg ha^{-1} for Tensor-II MIR, vis-NIR FS4-CP and vis-NIR FS4-ML, respectively. This confirmed again that the MIR spectrometer was best for nitrogen rate decisions. And the NIR and vis-NIR spectrometer-based recommendations performed slightly worse.

3.3.2. *Phosphorus fertilizer recommendation*

Fig. 5 shows the estimated phosphorus fertilizer rate (kg P ha^{-1}) required for a 7 t ha^{-1} yield target with the associated confidence interval estimated based on the error propagation from the prediction of Olsen P. Higher rates of P recommendation (>50 kg P ha^{-1}) were estimated better as there was a substantial agreement between the recommendation based on conventional Olsen P across the spectrometers. However, the disagreement substantially increased for recommended P rates below 50 kg P ha^{-1}, indicated by a considerable scatter of points away from the 1:1 line. This trend agreed well with the prediction pattern in Fig. 2 which had good predictions at low Olsen P values (and therefore high P fertilizer rates) but had longer error bars with deviation from the 1:1 line at higher Olsen P values (and therefore low P fertilizer rates). However, the overall RMSE of P recommendation was ranging from 10 to 12 kg ha^{-1} with very high negative bias (from −3.0 to −0.91) of estimation across the spectrometers, that could question the credibility of P fertilizer rate estimations using soil spectroscopic techniques. Besides, there were larger confidence intervals, irrespective of the spectrometers, at higher rates of phosphorus recommendations, indicating higher uncertainties and inefficiencies across the infrared spectrometers. When compared among spectrometers, the distance between the lower and upper bounds of the 95 % fertilizer P estimation difference between the spectrometers and conventional method appeared insignificant among the spectrometers. Besides, there was a trend of positive relationships among which may be attributed to the tendency to overestimate higher values of OlsenP by the spectrometers (Fig. 6). The 95 % P fertilizer estimation difference were –23.56 to 17.92, −21.23 to 18.98, −25.43 to 19.47 and −21.47 to −19.66 kg P ha^{-1} for vis-NIR FS4-CP, vis-NIR FS4-ML, NIR Neospec and MIR Tensor-II, respectively.

4. Discussion

4.1. *Prediction of soil property inputs for QUEFTS*

One of the sources of prediction imprecisions of soil properties by all spectrometers can be associated with the representativeness of the values in the training set for the specific soil properties (Brodský et al., 2013; Viscarra Rossel et al., 2016; Ng et al., 2020). This is due to the skewed distribution of the conventional analysis of some of the soil properties whereby the attribute ranges were not always well represented in training set with an adequate sample number. This can be observed in the scatter plot of Supplementary Fig.1 whereby samples were not evenly distributed across the PC score space. Hence, this might have created a smaller number of occasions for the model to train for those samples which are found in less dense space in the scatter plot. This result agrees with Viscarra Rossel et al. (2016) who reported prediction inconsistency due to the poor soil attribute value representation in the training set. In addition, Guerrero et al. (2016) reported that the inaccuracy of predictive models can be caused by the inadequacy of the soil libraries and a shortage of sufficient representative soil data. Brodský et al. (2013) reported a high deviation of measured versus predicted SOC at smaller values due to less representation in the training set. Hence, a representative calibration set is a vital component in soil

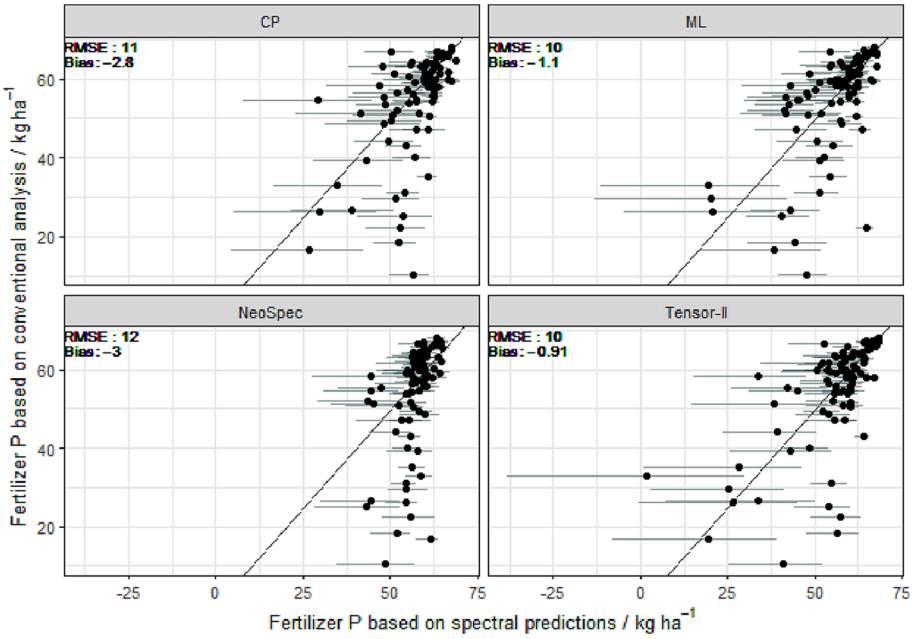


Fig. 5. Phosphorus fertilizer rate recommendation for a 7 t ha^{-1} maize target yield based on spectral (x-axis) and conventional (y axis) soil analysis. The statistics shown are the root mean square error (RMSE) and Bias for each spectrometer (FS4-CP -> FieldSpec 4 contact probe, FS4-ML -> FieldSpec 4 mug light, Neospec -> NeoSpectra Saucer, Tensor-II -> FTIR Bruker Tensor 27). The horizontal lines are the 95 % confidence intervals.

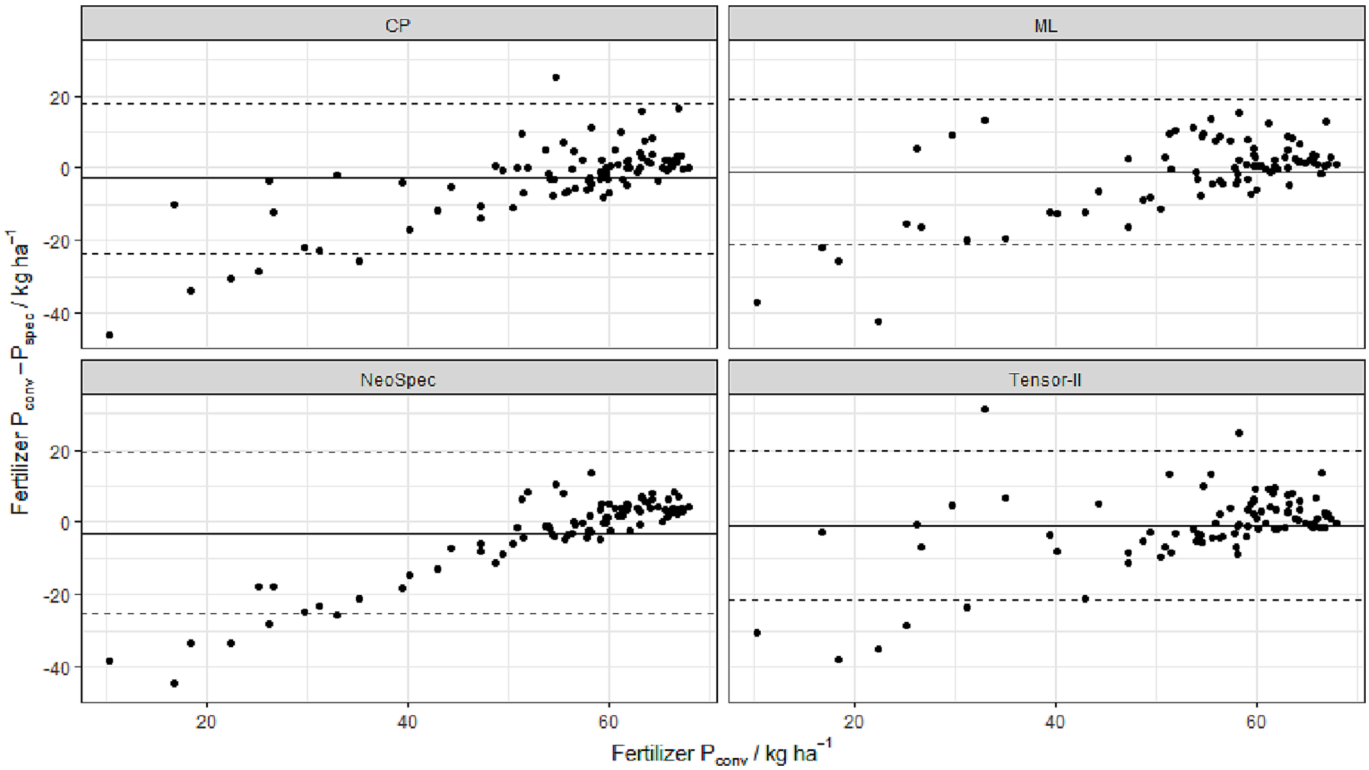


Fig. 6. Fertilizer P difference among the conventional and spectrometers (FS4-CP -> FieldSpec 4 contact probe, FS4-ML -> FieldSpec 4 mug light, Neospec -> NeoSpectra Saucer, Tensor-II -> FTIR Bruker Tensor 27). The dashed horizontal lines are the mean difference $\pm z^{(\alpha/2)}\sigma$. The horizontal line is the mean difference.

spectroscopy, and some of the prediction discrepancy might be solved with an optimized sampling strategy for the training set. Ng et al. (2020) also mentioned that large variations within the measured values without enough representation might yield an unstable model, which affects the soil nutrients predictions.

In general, the model prediction parameters for most of the QUEFTS inputs did not vary much between the spectrometers, though the prediction performance varied among soil properties whereby the prediction performance of Olsen P was the poorest of all. Several studies concluded that infrared spectroscopy is not satisfactory to predict plant available P when testing the predictive models with an independent test set (e.g., Pätzold et al., 2020). And the prediction performances in all the visible and infrared regions for the soil properties considered were comparable or better than reported by other researchers (Gates, 2018; Ng et al., 2020; Rodríguez-Pérez et al., 2021; Vestergaard et al., 2021; Wijewardane et al., 2018). However, there were differences between the spectrometers and the prediction accuracies for most of the soil properties were best in the MIR and vis-NIR range as compared to the NIR, especially for Olsen P and SOC as a result of the missing wavelength range (Bellon-Maurel and McBratney, 2011). Our result is in consent with the findings of Zelikman and Carmina (2013) who reported lower performance of the NIR range to predict SOC Barra et al. (2021) identified in their review paper that most comparisons favoured the MIR spectroscopy over the vis-NIR or NIR spectroscopy with regards to prediction accuracy and consistency although some studies also found better performance of NIR for some soil properties. However, Li et al. (2022) advised that NIR is the most cost effective method for SOC analysis, compared with MIR spectroscopy and dry combustion, and assuming > 250 samples per day had to be analyzed. They recommended that vis-NIR spectroscopy was cheaper, accurate and had a large capacity for quick measurements.

Besides these factors, the complexity of acquiring the spectra could be added to the evaluation of different spectrometers, especially for the application in developing countries. Portable NIR spectrometers could allow field-based application whereas bench-top MIR spectrometers require proper laboratories and liquid nitrogen to cool the light source. MIR spectrometers also need fine milled samples whereas NIR and Vis-NIR spectrometers give good results with sieved soil or even in-field scanning (this study and Breure et al., 2021). And finally, the initial equipment cost is another argument, clearly favouring the low cost NIR equipment used in our study. Therefore, our findings suggested that the small NIR spectral range covered by the NeoSpec had little negative effects on the prediction accuracy for the QUEFTS inputs even though the overall prediction performance was in the order of MIR > vis-NIR > NIR spectrometers. Hence, NIR seems to have a comparative advantage in generating relevant soil information regarding prediction precision, cost effectiveness and ease of application.

4.2. *Fertilizer determination through soil spectral tools by coupling with QUEFTS*

Knowledge of relevant soil characteristics is a vital component to advise precise nutrient management adjusted to local conditions and different crop types. Consequently, soil testing has been widely accepted and used as a tool for rational fertilizer use, helping to achieve optimal yields with high nutrient use efficiency and minimized losses to the environment. Moreover, soil-test and crop response based empirical models such as the QUEFTS model (Janssen et al., 1990; Haefele and Wopereis, 2005; Sattari et al., 2014; Yang et al., 2017) or yield response functions (Dhakal and Lange, 2021) have been developed for many cropping systems, using general soil characteristics, nutrient availability tests and/or observed crop responses to applied nutrients as input parameters. These approaches progressed overtime to assess the soil fertility status and recommend suitable and economic nutrient rates through inorganic fertilizer and organic manure for different crops and cropping systems.

However, there are considerable challenges in many countries in getting soil test results in time and at the required scale with

conventional soil testing methods. Hence, applicability of easy soil testing methods and harmonized approaches of fertilizer recommendations could enable instant site-specific fertilizer management, enhancing overall productivity and improved nutrient use efficiency. Employing soil spectroscopic techniques with empirical fertilizer determination could be a breakthrough to alleviate the existing low productivity and nutrient use efficiency through informed decision in developing countries where technologies and information are scarce. Though some researchers argued the non-existence of a standard functional form to evaluate optimal fertilizer recommendation (Dhakal and Lange, 2021), we considered that the QUEFTS model could be a candidate platform to harmonize efforts towards fertilizer recommendations with low costs, especially when coupled with efficient soil testing. The QUEFTS model is a versatile soil-crop-fertilizer model that demands very few inputs (four soil properties and calibrated soil-crop-fertilizer parameters) to derive site specific nutrient rates for optimized nutrient use of various crops (maize, wheat, rice, oil palm, manioc, and cotton) and for both tropic and subtropic environments.

In this research, the resulting recommendation for NP fertilizer for the attainable yield (70 % of water limited potential yield) using soil spectroscopic techniques coupled with the QUEFTS model agreed well with the nutrient rates reported by Kenea et al. (2021) and ten Berge et al. (2019) for maize in the soil sample regions. Our findings revealed that the error propagated from the spectral training models was not further exacerbated by the QUEFTS model and parameters although the relative marginal uncertainties for the recommendations increased. This signified the feasibility of predicted soil inputs to be used in the QUEFTS approach. Our results indicated that spectroscopic methods predicted the QUEFTS-relevant soil properties with reasonable accuracy, confirming that a site-specific fertilizer recommendation could be derived efficiently and much faster if compared to the conventional method. Ng et al. (2022) had also proposed a categorical nutrient recommendation based on the vis-NIR or NIR as well as MIR region of the electromagnetic spectrum to alleviate the challenges of cost, complexity, and accessibility of soil testing in developing countries.

When we compared the spectrometers for their efficiency, longer confidence interval bars, revealing higher uncertainties associated with the recommendation, were observed for total N predictions when using NIR and vis-NIR ranges rather than MIR spectra, though most points fall on or close to the 1:1 line when compared with the conventional nitrogen fertilizer determination. Besides, the fertilizer N difference was in a range of acceptable estimation which ranged between −8 to 8 kg N ha^{-1} for the NIR which was the least performing spectrometer. In contrast, longer confidence intervals, which were comparably similar for all soil spectrometers, were observed for P fertilizer recommendations and the points tended to be underestimated for P rates below 50 kg ha^{-1} with wider estimation differences with the conventional method. The MIR spectrometer was, in general, more efficient and effective spectrometer when compared to the vis-NIR and NIR spectrometers for use in fertilizer recommendation. However, its current complexity and cost to use for such purposes for developing countries could be impractical and the vis-NIR spectrometers, though portable, are still costly with a minimum or no variation in prediction performance when compared to the NIR spectrometer. In contrary, the NIR spectrometer is cheaper, portable and has very low running cost which can be used in the field and in low-income countries. This result ascertained that the cheaper, flexible to use and handheld NIR can contribute a lot in access to soil information for informed decision to improve productivity while decreasing fertilizer cost which ultimately improve livelihood of the farmers.

To summarize, the spectroscopic methods followed were efficient and effective for N fertilizer recommendations, and we could not evaluate their use for K fertilizer estimation because all soils analyzed had a high K supply (but the prediction of exchangeable K was promising). The estimation of phosphorus fertilizer rates with soil spectroscopic techniques was unsatisfactory in precision, often overestimating the P fertilizer rate on soils with a good P supply. Its application for this purpose needs further investigation and consideration of larger and better-balanced calibration sets and/or improving the predictive model approach.

5. Conclusions

The study evaluated commercially available spectrometers in the vis-NIR, NIR and MIR for their effectiveness, efficiency and usefulness for analyses of soil properties important for fertilizer decision tools. In a second step, the predicted soil data was coupled with the QUEFTS model to evaluate the effect of uncertainty on potential fertilizer recommendations. Spectrometer-wise, the MIR and the portable vis-NIR were more costly than the handheld NIR. Besides, the benchtop MIR requires extended time for sample preparation (i.e., milling and sample loading). We showed that fertilizer decision for nitrogen and phosphorus can be made by use of spectra generated from spectrometers in the NIR, vis-NIR and MIR range in conjunction with the QUEFTS and soil-test based fertilizer models for site specific fertilizer application. The confidence interval indicated that the uncertainty could be acceptable than a blanket or uninformed decision for both environmental, productivity and input cost perspectives. Specifically, the NIR spectrometer would be applicable being low-cost and ease of applicability than the expensive benchtop MIR and vis-NIR spectrometers in the low-income countries whereby the estimation of nitrogen and phosphorus fertilizer were proven comparable to other expensive methods to generate soil information. Our result didn't include any comparison of the outcome of the recommendation with crop data. Hence, further study might be appropriate to evaluate the precision of the nitrogen and phosphorus fertilizer estimated by soil spectroscopic techniques with QUEFTS model with crop response.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Author Contributions

T.G.A., S.M.H, R.S., F.K., R.C. and K.H. conceptualized the study, and

acquired and administered project funding. T.G.A. and T.B. contributed to data analyses, including method development, data visualizations and data interpretation. T.G.A wrote the primary draft of the paper with editing and reviewing inputs from other authors.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.geoderma.2023.116397.

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