



Prediction of Potassium (K) Content in Soil Analysis Utilizing Near-Infrared (NIR) Spectroscopy

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ABSTRACT

The relationship between NIR spectroscopy spectral absorbance and potassium (K) is studied as a representative factor for analysing soil's nutritional content. To determine the potassium content of soil samples without resorting to intrusive and time-consuming chemical analysis techniques, NIR spectroscopy sampling techniques have been tested. Spectrum absorption data from 900 nm to 1600 nm were discovered to correspond with potassium values and were then analysed using a number of pre-processing procedures. Five techniques, Multiplicative Scatter Correction (MSC), Multiplicative Scatter Correction using Common Amplification (MSSCA), Multiplicative Scatter Correction using Common Offset (MSCCO), Detrending (DT), and Mean Normalization (MN), have been identified as the most effective. Using the Partial Least Squares Regression (PLSR) model, both calibration and prediction data are evaluated. In the end study, the MSCCA method was determined to be the most effective pre-processing method for both calibration and prediction outcomes, with R^2 values of 0.9998 for calibration and RMSE values of 0.0600 for prediction. Utilising PLSR model and the MSCCA preprocessing method, the relationship between NIRS absorbance data and potassium may be determined. Consequently, we may infer that the NIRS approach can be utilised to detect amount of potassium in soil analysis employing a less time-consuming, non-invasive, and labour-intensive sampling technique.

1. Introduction

Many facets of plantation, fertilisation, and harvest have been known and enhanced in modern agriculture, including planting, fertilisation, and harvesting. Watching and analysing soil samples is among the most significant technologies that have developed significantly. Researchers are increasingly using near-infrared (NIR) spectroscopy to analyse soil parameters because they recognise its benefits over soil analysis laboratory standard techniques [1-5]. The determination of

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soil parameters traditionally relies on field sampling and laboratory investigations, which can be both resource-intensive and time-consuming, encompassing chemical analysis [6-10]. NIR spectroscopy is a low-cost, non-invasive, and time-saving method of analysis that requires minimal sample preparation. Moreover, many calibrated characteristics of the same samples can be analysed concurrently inside a single spectral analysis [11].

NIR spectroscopy ranges from 780 nm to 2500 nm in wavelength. Furthermore, the spectral regions in which soil exhibits absorption properties are characterized by overtones associated with the stretching and bending vibrations of chemical bonds, such as C-C and O-H [12].

Potassium (K) in the soil, on the other hand, is one of the most frequently recognised features that combat soil nutrient deficit. K₂O exists in the form of potassium chloride (KCl), potassium sulphate (K₂SO₄), potassium nitrate (KNO₃), and potassium magnesium sulphate (KMgSO₄) in the soil (K₂SO₄ 2MgSO₄). Potassium promotes the growth of cells, roots, stems, and overall growing mechanisms, and as plant size increases, so does the demand for potassium. Potassium shortage concurrently limits a plant's development [13]. The primary objective of this study was to investigate the potential of NIR spectroscopy as a viable alternative to the conventional approach in assessing soil parameters, specifically potassium concentration. The study aimed to assess the feasibility of employing NIR spectroscopy as a rapid, cost-effective, and non-invasive technology for this purpose. The performance of the Partial Least Square Regression (PLSR) model while also exploring the impact of several data pre-processing techniques will also be examined in this study to estimate the potassium concentration. Finally, determining the NIR spectroscopy wavelength range has a strong correlation with potassium characteristics.

2. Methodology

2.1 Sampling

For the soil sample, 70 readings are taken from seven distinct types of soil gathered from various agricultural plantations in northern Malaysia, including mango, chili, papaya, and okra. The sample comprises healthy plants and demonstrates secondary characteristics, including a shorter stem, yellowing leaves, and fewer leaves. The aggregation of multiple soil types yields a wide range of data sets that can be utilized for the purpose of data correlation [14]. In general, plants that exhibit adequate levels of essential components are more suitable for potassium uptake compared to plants that are weak in certain elements [15].

A soil sample is extracted from a depth of 5 to 10 centimetres beneath the crop layer using a drill equipped with spiral bits specifically designed for soil sampling, as depicted in Figure 1. A systematic sampling approach was employed to collect random samples at several sampling sites located in northern Malaysia over the period of December to March 2021, which corresponds to the hot and dry season. The rise in temperature and wind velocity during this period creates favourable conditions for sampling due to the natural evaporation of soil moisture, which results in the concentration of residual nutrients within the soil [16,17]. Every soil sample is securely enclosed within a plastic bag and appropriately labelled with precise details like the time, date, and specific location.

The acquired sample is processed in the laboratory at the suitable time by undergoing a sieving process using a 1-mm sieve, subsequent to being crushed using a mortar and pestle [18]. Next, the sample is divided into two distinct groups in order to perform calibration and collect spectral data. Following this, the specimens are retained into a labelled petri dish, subsequently undergoing a 48-hour air-drying process to remove any residual moisture that may potentially disrupt the spectral analysis conducted by the NIR spectrometer [19].

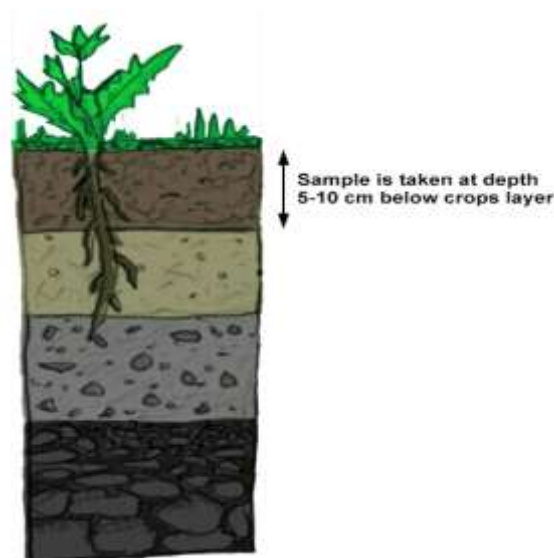


Fig. 1. The cross section of the soil reveals the portion of the soil that is sampled

2.2 Calibration and Data Measurement

The potassium concentration in the soil, specifically in the form of potassium (K) ions, was determined using a Hanna HI83300 Multiparameter Photometer as the calibration data. The instrument working in the visible spectrum occupies a measurement range spanning from 0.0 to 30.0 mg/L, exhibiting a resolution of 0.1 mg/L. The HI83300 instrument has the option of multiparameter mode; however, it is necessary to acquire a separate chemical reagent set from Hanna equipment for each specific parameter that is being measured. In this study, a total of 100 potassium (K) reagents were gathered for the purpose of conducting 100 experiments. The reagent consists of many chemicals that enhance the detection of potassium in soil samples.

The DLPNIRscan Nano Evaluation Module (EVM), which is made for the study of spectral data, will be used for the evaluation of absorbance. This module is manufactured by Texas Instruments, a company based in Texas, USA. In contrast to the reflectance phenomenon observed when light is incident upon the surface of soils, NIRscan outcomes are presented in terms of absorption. For each data readout, the absorbance in the spectrum is calculated and measured between 900 nm and 1700 nm [20]. Prior to conducting the test, it is imperative to calibrate NIRscan by employing Polytetrafluoroethylene (PTFE) compound. This calibration procedure ensures that the instrument achieves optimal reflectance and minimal absorbance, hence facilitating the attainment of accurate results with minimal calibration errors [21].

In order to achieve a comprehensive reading for each soil sample, a total of 10 random measurement points is acquired using NIRscan technology for each individual petri dish containing soil samples, as depicted in Figure 2. These individual measurements are subsequently combined and averaged to obtain a single averaged reading for each soil sample. As a consequence of the limited quantity of reagents accessible for the HI83300, measurements are performed singularly for each sample, allowing for a maximum of 100 samples per reagent batch. After the calibration process and measurement of spectral data, a spectrum containing the absorbance response of each soil sample is presented for analysis. The purpose of examining this spectrum is to identify any trends and detect any measurement errors.

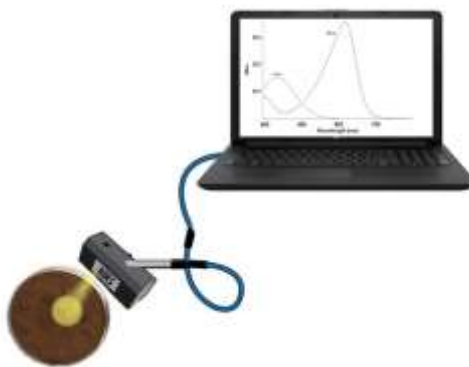


Fig. 2. NIR spectrometer taking the reading of soil samples in petri dish

2.3 Pre-Processing Technique

To minimize data interruption and noise, the earliest and final 50 nm of the initial absorbance spectra were eliminated, leaving the remaining 950 nm to 1650 nm of the total NIR spectrum wavelength [22]. Additionally, negative, null, and severe data are eliminated from the collected data through a pre-treatment procedure as to improve the PLSR model's performance. After rigorous testing and analysis, five preprocessing approaches were chosen from a pool of several. The Multiplicative Scatter Correction (MSC), Multiplicative Scatter Correction using Common Amplification (MSSCA), Multiplicative Scatter Correction using Common Offset (MSCCO), Detrending (DT), and Mean Normalization (MN) techniques are chosen to process the spectral data in this study due to their superior performance during PLSR model testing. These pre-processing techniques have been compared to discover the optimal pre-processing method. The conclusion will be drawn based on the evaluations of the coefficient of determination (R^2) and root mean square error (RMSE).

2.4 Prediction Model

The primary focus of the model lies in making predictions for answers rather than explicitly striving to recognize the fundamental relationship between variables. Selection of X and Y-scores is conducted in order to maximize the strength of the association between consecutive sets of scores, within the constraints of the given circumstances. This approach can be seen as a form of redundancy analysis that aims to identify the direction in the factor space that is associated with a high level of variability in the answers. Additionally, it introduces a bias towards the factors that can be perfectly predicted [23].

PLSR is a statistical technique that integrates and synthesizes the principles of Principal Component Analysis (PCA) and Multiple Regression (MR) in order to make predictions or analyse a set of dependent variables using a set of independent variables or predictors. The process of recovering a prediction involves extracting it from a set of orthogonal components known as latent variables (LVs), which are selected based on their high predictive potential. The spectrum matrix X and the response matrix Y are generated using PLSR to create the orthogonal basis of LV, which is oriented in the direction of the maximum correlation between the two. The maximum number of LV allowed for this study is 10, as any number higher than that would indicate non-existent data [24].

In order to validate the link between potassium calibration data and NIR spectral data, PLSR will therefore be preferred as the prediction model. The complete sample data is separated into two groups at random—75% for calibration and 25% for prediction—before the calibration model is

created. The aforementioned ratio has been identified as the optimal ratio for the examination of prediction models in previous research [25]. The prediction set validates the models while full cross-validation is used to assess the validity of the calibration models and avoid overfitting the graph. The software 'The Unscrambler X' (version 10.4) was utilized to conduct and evaluate PLSR analysis and preprocessing techniques.

3. Results

The spectral plot depicted in Figure 3 illustrates the results of a comprehensive analysis involving 70 soil samples from seven distinct soil types. The analysis was conducted within the near-infrared (NIR) spectral range, specifically spanning from 900 nm to 1700 nm. However, it is worth noting that the observed correlation is limited to the range of 950 nm to 1650 nm. The graph illustrates the relationship between absorbance and wavelength across different soil samples. The graph illustrates a significant increase in soil sample absorption within the wavelength range of 1330 nm to 1650 nm. Subsequently, the obtained absorbance values were subjected to analysis using a predictive model in order to assess the relationship between absorbance and potassium data readings.

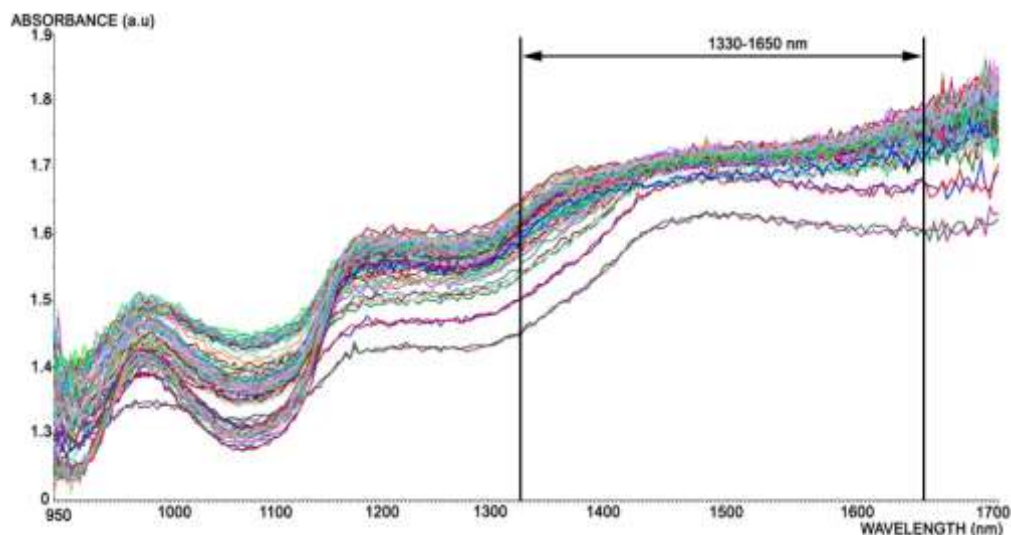


Fig. 3. The spectral graph depicts the absorbance of potassium levels in soil sample

As a result, the PLS regression prediction model is used to assess the potassium and spectral absorbance data, and the best pre-processing method is then chosen. Five pre-processing methods—MSC, MSCCA, MSCCO, DT, and MN—out of 20 have generated interest. In Table 1, a novel pre-processing method that has been tried out is offered along with the evaluation of potassium data and spectral absorbance. Each of the seven different types of soil samples is combined and tested using the overall data that is produced after the evaluation of the results.

Table 1
 PLSR evaluation with optimum pre-processing technique

Pre-processing technique	Calibration		Prediction	
	R ²	RMSE	R ²	RMSE
Multiplicative Scatter Correction Common Amplification (MSCCA)	0.9999	0.0201	0.9999	0.0600
Multiplicative Scatter Correction (MSC)	0.9999	0.0024	0.9996	0.0404
Multiplicative Scatter Correction Common Offset (MSCCO)	0.9997	0.2961	0.9978	0.8677
Detrending (DT)	0.9994	0.4088	0.9973	0.9150
Mean Normalization (MN)	0.9997	0.1653	0.9973	0.5301

The selected absorbance spectral is spilled into a 7-range section that is distributed evenly, and section 7th (1330 nm to 1650 nm) is chosen as the observation range to be analysed because this range shows a highly anticipated correlation for both data. For this analysis, R^2 and RMSE will be the performance benchmark for the correlation between potassium data and spectral absorbance data. Despite R^2 , the correlation performs best between 0.70 and 0.90, or even better, if it's possible, closer to 1.00. On the other hand, the best RMSE are assessed in the 0.10 to 0.90 range, or even better, closer to 0.00 [26].

According to the data presented in Table 1, the MSCCA technique exhibits the highest level of anticipated and intended calibration, as evidenced by its R^2 values of 0.9999 and RMSE of 0.0201. Significantly, the prediction outcomes fall within the optimal predicted range, as depicted in Figure 4. Specifically, the R^2 value remains consistent with the calibration findings at 0.9999. However, it is worth noting that the RMSE of 0.0600 is marginally higher in comparison to the calibration results. This study demonstrates a strong correlation between the predictive capability of the technique and the stated spectral absorbance values for potassium. The association between the calibration and prediction of potassium and spectral data is depicted in Figure 4 to 8. Predicted data are shown by the red dot, whereas calibrated data are represented by the blue dot.

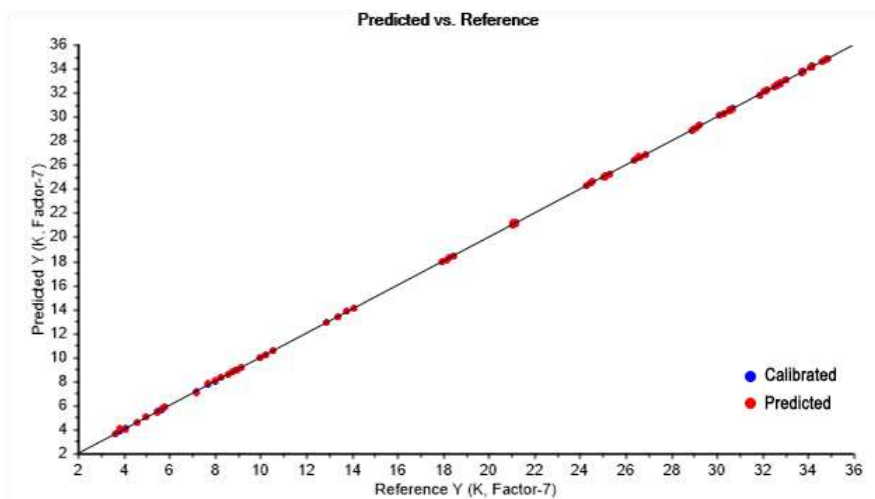


Fig. 4. PLSR prediction using MSCCA technique

As we can observe from Figure 5, the MSC technique has likely achieved a proportional linearity plot with MSCCA and MSCCO techniques. With the values of 0.9999 for R^2 and 0.0024 for RMSE, it is considered the highest performance for calibration RMSE of the overall technique. Looking at the prediction, it successfully achieves R^2 values of 0.9996 with RMSE values of 0.0404. Based on the predicted values for the MSCCA method in the 2nd listing, the aim is nearly accomplished.

In comparison, the MSCCO technique, as depicted in Figure 6, has superior calibration performance, as evidenced by its R^2 values of 0.9997 and RMSE values of 0.2961. In comparison to the predicted outcome, the MSCCO technique demonstrated the third highest performance, with R^2 values of 0.9978 and higher RMSE values of 0.8677.

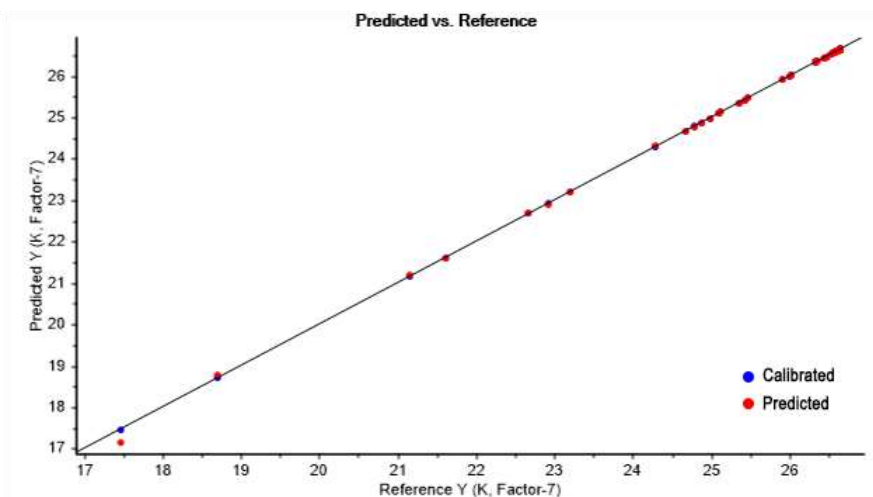


Fig. 5. PLSR prediction using MSC technique

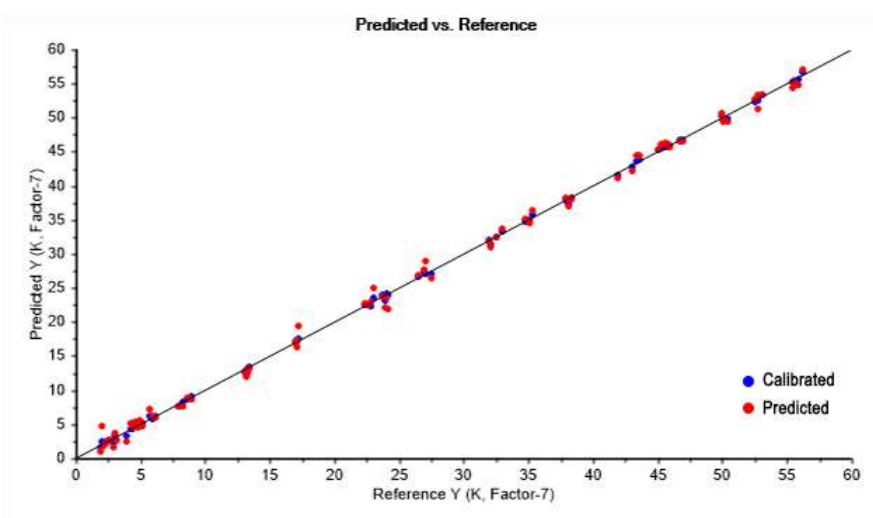


Fig. 6. PLSR prediction using MSCCO technique

From Figure 7 and 8, it is quite probable that the observed DT and MN approach yield similar R^2 results. The DT technique demonstrated high calibration performance with R^2 values of 0.9994 and RMSE values of 0.4088. Similarly, for prediction, the DT technique exhibited strong performance with R^2 values of 0.9973 and RMSE values of 0.9150. In a similar vein, the MN method R^2 has been assessed to be 0.9997 and the RMSE to be 0.1653 for the purpose of calibration. In terms of prediction performance, this demonstrated R^2 values of 0.9973. However, it is worth noting that the RMSE for this technique is lower compared to the RMSE values obtained from the DT and the MSCCO prediction methods, specifically at a value of 0.5301.

Based on the findings, it can be concluded that the MSCCA technique outperformed the other four techniques examined in this study in terms of preprocessing for the correlation analysis of potassium and spectral absorbance data. As a recommendation for future research, it is advisable to incorporate other variables into the observation process that may potentially impact the performance of the prediction model. These variables include the chemical makeup of the subject under study, as well as the quantity and specific type of fertilizer utilized. In addition to this, it is anticipated that a greater quantity of samples will enhance the correlation and precision of the predictive model.

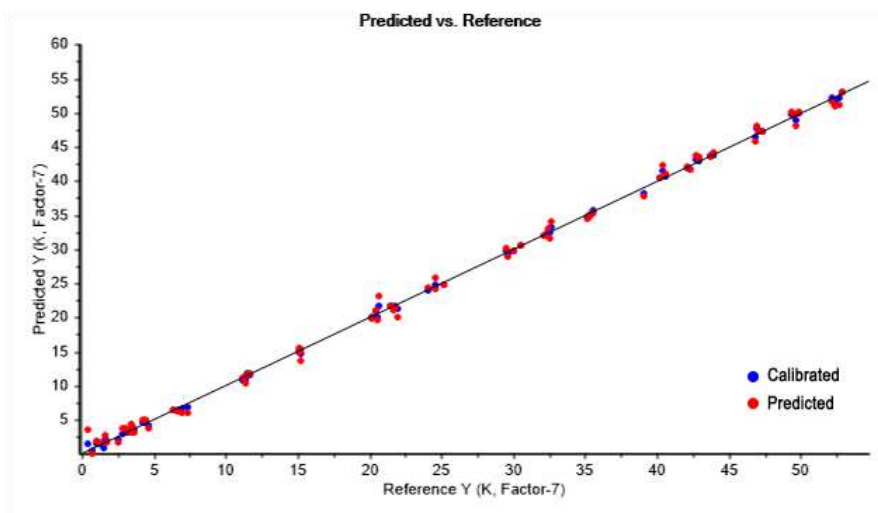


Fig. 7. PLSR prediction using DT technique

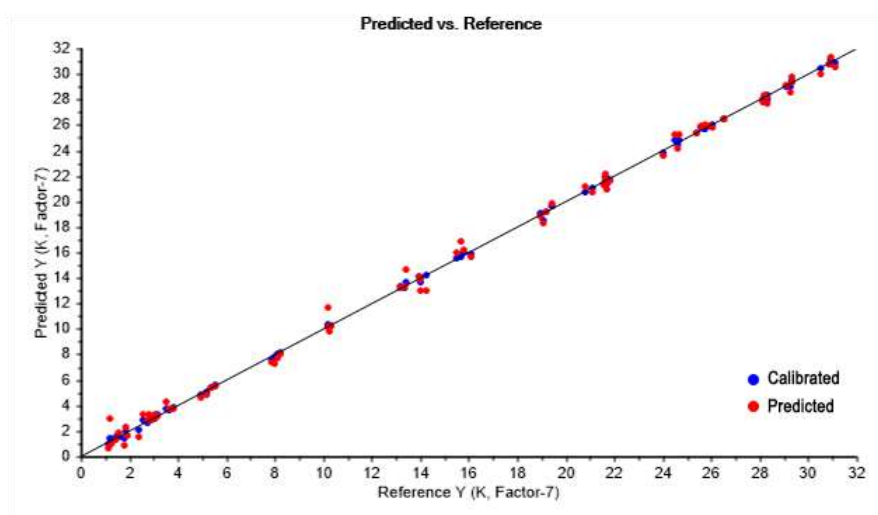


Fig. 8. PLSR prediction using MN technique

4. Conclusions

In conclusion, after conducting thorough testing and observation, it has been established that the MSCCA pre-processing technique is the optimal method for correlating potassium data with spectral absorbance data of soil samples in the context of soil analysis. Furthermore, it can be inferred that the utilization of NIRS in the analysis of soil enables a more efficient identification of potassium concentrations. This is achieved by the implementation of a sampling method that is both time-saving and non-invasive, hence reducing the hassle associated with traditional approaches. This process is further enhanced by the incorporation of a pre-processing technique known as MSCCA and a PLSR model. The NIRS device is a valuable instrument for future research in soil analysis, since it allows for the effective observation of numerous nutrients that may be recommended for examination.

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