24-025

Determination of Incombustible Content with Portable Spectrometers Using Chemometric Modelling: Preliminary Results

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ABSTRACT

Inertization of coal dust with stone dust is a common control implemented within underground coal mines to mitigate the hazard of a coal dust explosion. To achieve adequate inertization, the total incombustible content (TIC) of the coal/stone dust mixture is required to meet certain percentages depending on the risk and relevant legislation. Current methods for determining the TIC of a mixture involves laboratory analysis, colorimetric comparison, or the use of portable instruments. This paper provides preliminary analysis of determination of a sample's TIC in real-time with chemometric modelling, using portable instruments employing near-infrared (NIR).

INTRODUCTION

The development of portable instrumentation for roadway dust testing in underground coal mines is not a recent concept. The National Institute for Occupational Safety and Health (NIOSH) had developed a commercial product called the Coal Dust Explosibility Meter (CDEM) in the early 2000's, which was in commercial use by [1]. The CDEM instrument worked on the broadband infrared reflectivity (IR) of a sample and was calibrated on Pittsburgh coal and stone dust samples with up to 80% total incombustible content (TIC). The device uses a photodiode to evaluate the concentration of total incombustibles present in a sample. An evaluation of the CDEM for Australian mining operations recommended its implementation [2]. However, in the study, the comparison of the CDEM was only investigated against laboratory results and the analysis did not consider natural incombustible content of the coal samples tested within Australia. In addition, the device would have had to be modified to allow analysis in accordance with Australian legislative requirements. In 2015, the device was evaluated in the field for use in Australian coal mines [3]. Several limitations were observed, including poor reference sample design for Australian coal mines, unfriendly calibration methodology, lack of certification for intrinsic safety and sensitivity of the measurement to moisture within the sample requiring coal sample to be dried. This led to the recommendation not to adopt the NIOSH device in its existing state as a tool for rapid analysis of stone dust compliance in Australia.

For Queensland, Australia, the Recognised Standard 5 (RS5) stipulates the requirements for incombustible content (IC) per zone and how the testing methodologies are to be conducted [4]. RS5 allows for a portable instrument to be used for the analysis of roadway dust samples if it is as accurate as laboratory analysis; however, RS5 does not stipulate the accuracy required for laboratories undertaking the analysis. This poses a challenge with how accuracy is reported not only between laboratories but also due to the fundamental differences of the tests (gravimetric vs spectrometry). For instance, CDEM provides qualitative results (Go/No-Go) while laboratories provide a quantitative analysis. In addition, the CDEM specifications state that the accuracy is ± 2 %, however, this is only true when using completely dried samples. One percent (1%) moisture can drop the IC readings by as much as 7% [1].

The rapid development of spectral sensors within the last decade has resulted in numerous portable spectrometers being developed and brought to market. This has allowed for the identification of materials in the field rather than the laboratory. More recently, advances in regression modelling along with higher resolution sensors now allow for portable quantitative analysis of materials. For instance, portable X-ray fluorescence has been used for the analysis of ash content in coal [5]. Recent advances in micro-electro-mechanical systems (MEMS) have allowed rapid technological advancement of miniaturized and rugged spectrometers while the advancement in the field of machine learning, and particularly chemometrics, has allowed complex analysis of samples through spectroscopy to be applied to everyday analysis. The advantages of using MEMS sensors is that accurate and rapid material testing can be conducted with handheld apparatus, at very low power allowing the potential for intrinsically safe design to be viable. Additionally, the use of near-infrared (NIR) spectrum sensors brings a unique advantage over photodiodes as it can detect moisture within the NIR region.

Simtars is currently undertaking a viability study of portable spectrometers for the rapid analysis of TIC as part of a Coal Health and Safety Trust funded project (No. 20663) under laboratory conditions. The project is focusing on devices available on the market, along with the application of machine learning algorithms to determine TIC.

In this paper, the preliminary analysis to determine the TIC of samples in real-time with chemometric modelling using a portable instrument system employing near-infrared spectroscopy is presented. The classification model used demonstrated a high accuracy of 76.92% for Category 2 (TIC = 70%–80%), however, its overall accuracy of 56% requires further analysis with the main difficulty encountered during the classification within the grouping of Category 1 (TIC < 70%).

METHODOLOGY

Spectrometer

The Stellarnet NIR ADK portable spectrometer was used for this study. Utilizing a crossed Czerny-Turner optical system, this NIR spectrometer operates within a wavelength range spanning from 900 to 1700 nm, with a resolution of less than 5 nm and wavelength accuracy of less than 0.25 nm. It uses near-infrared light to analyze the vibrational transitions within molecules, especially O-H, C-H, and N-H bonds.

Sample Preparation

To compile a chemometric dataset, one hundred (100) coal samples from Australian mines (Queensland and New South Wales) were randomly selected for analysis. These 100 coal samples underwent proximate analysis for coal quality: moisture, ash, volatile matter, and fixed carbon contents. The results of the statistical analysis of the coal quality per region (Queensland and New South Wales) are summarized in Table 1. Levene Test and the One-Way ANOVA determine if there are significant differences in independent groups, providing insights into group variability and potential statistical significance. Both the Levene Test and the One-Way ANOVA yielded low test statistics and high p-values for all coal quality parameters, except for moisture. Specifically, the p-values for these parameters were consistently greater than 0.05, indicating no statistically significant variance among regions [6]. This suggests that the 100 coal samples were drawn from a similar sample group across Queensland and New South Wales. The notable difference observed in moisture content between the two regions, as indicated by a p-value less than 0.05, may be attributed to the preservation of the coal samples, considering that these samples originated from a span of 20 years.

Table 1. Statistical Analysis of Coal Quality by Region

Coal Quality	Levene Test	One-Way ANOVA
Ash	0.21, p=0.65	0.19, p=0.67
Moisture	7.20, p=0.009	4.60, p=0.04
Volatile Matter	0.01, p=0.93	1.41, p=0.24
Fixed Carbon	2.32, p=0.13	0.16, p=0.69

The stone dust dosing regime was calculated based on a polymodal distribution centered around the three regulatory limits of 70%, 80% and 85%, with a standard deviation of 5%. This polymodal distribution was then randomly applied to all coal samples resulting in the total of 300 coal/stone dust samples with varying total incombustible content (TIC) values from the polymodal distribution. The spread of the TIC in samples is displayed in Figure 1. For quality assurance purposes, the TIC values were measured by two independent laboratories and the results showed good correlation.

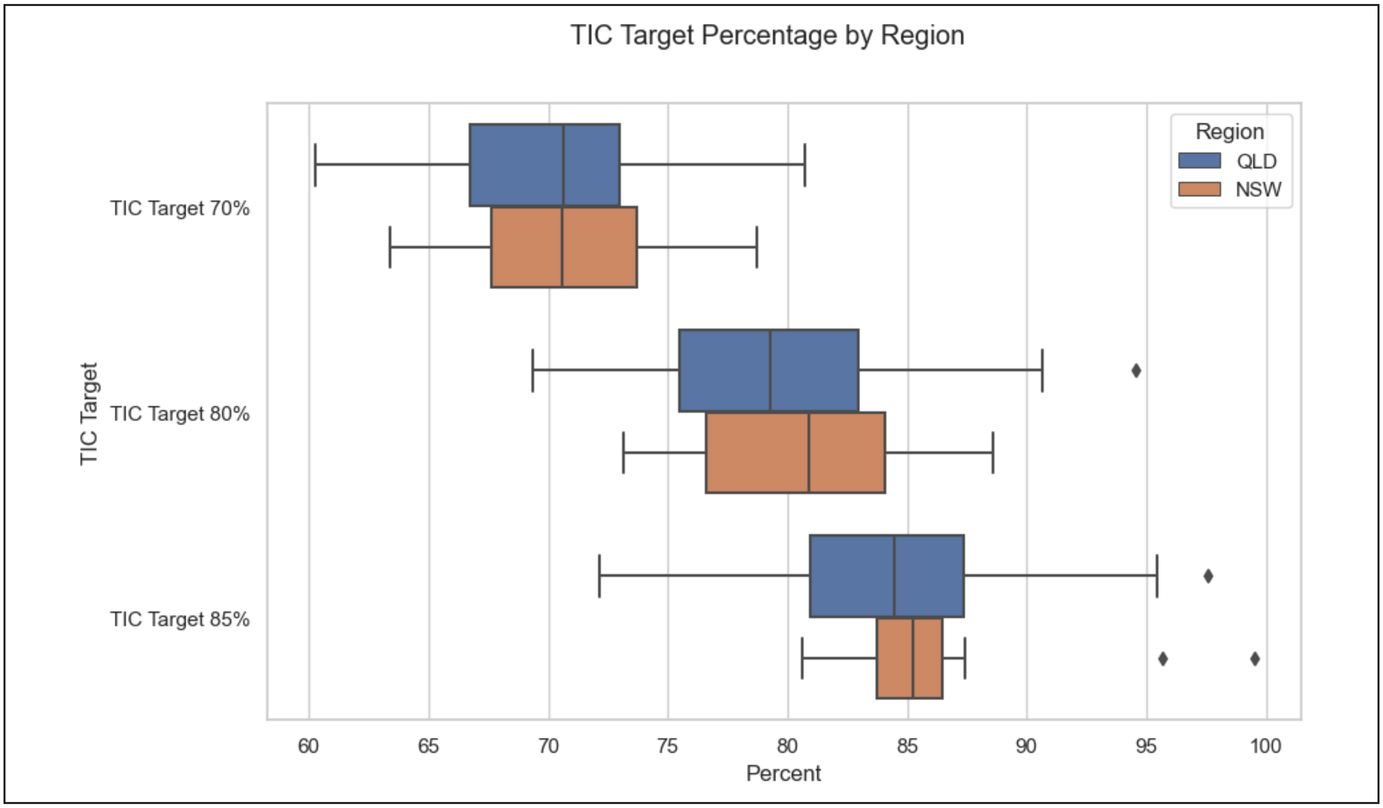

Figure 1. TIC Target by Region

NIR Spectral Data Acquisition

Data acquisition commenced with scanning of coal/stone dust samples using the StellarNet NIR ADK device. A total of 400 samples were scanned for analysis: 100 coal samples and 300 coal/stone dust samples. Spectral recording was undertaken using the instrument's interface. All the samples subjected to scanning were systematically categorized into five distinct groups, as summarized in Table 2. The raw spectra of the scanned samples are presented in Figure 2. The spectral data was then pre-processed using a combination of MATLAB and Python for the subsequent machine learning analysis. Note that the spectra of the 100 coal samples were removed as they were not used for model development. The data pre-processing process included adjustments of wavelength range, scatter correction [7], smoothing [8] and Tukey's Fence cleaning [9] of raw spectral data. The pre-processed spectra are presented in Figure 3.

Table 2. Categories of Coal and Coal/Stone Dust Samples

Category	Internal Actual TIC	Number of Samples
1	<70%	28
2	70%–80%	116
3	80%–85%	78
4	>85%	78
Coal	Original Coal	100

MODEL DEVELOPMENT AND EVALUATION

Machine learning techniques were employed to evaluate the data after the completion of the data pre-processing phase towards the development and evaluation of the models, which included both the regression and classification models. The spectra dataset underwent a random partitioning into two distinct subsets: a training set, comprising 227 spectra (representing 90% of the data), and a test set, encompassing 25 spectra (equivalent to 10% of the data). The training set served as the foundation for the construction and refinement of machine learning models through the utilization of MATLAB R2022b. Subsequently, the test set was employed to assess the performance and generalization capabilities of the developed models.

Regression Models

A comprehensive assessment of various regression models was conducted, including Linear, Support Vector Machine (SVM), Gaussian Process Regression (GPR), and Neural Network (NN) with the objective of finding the most

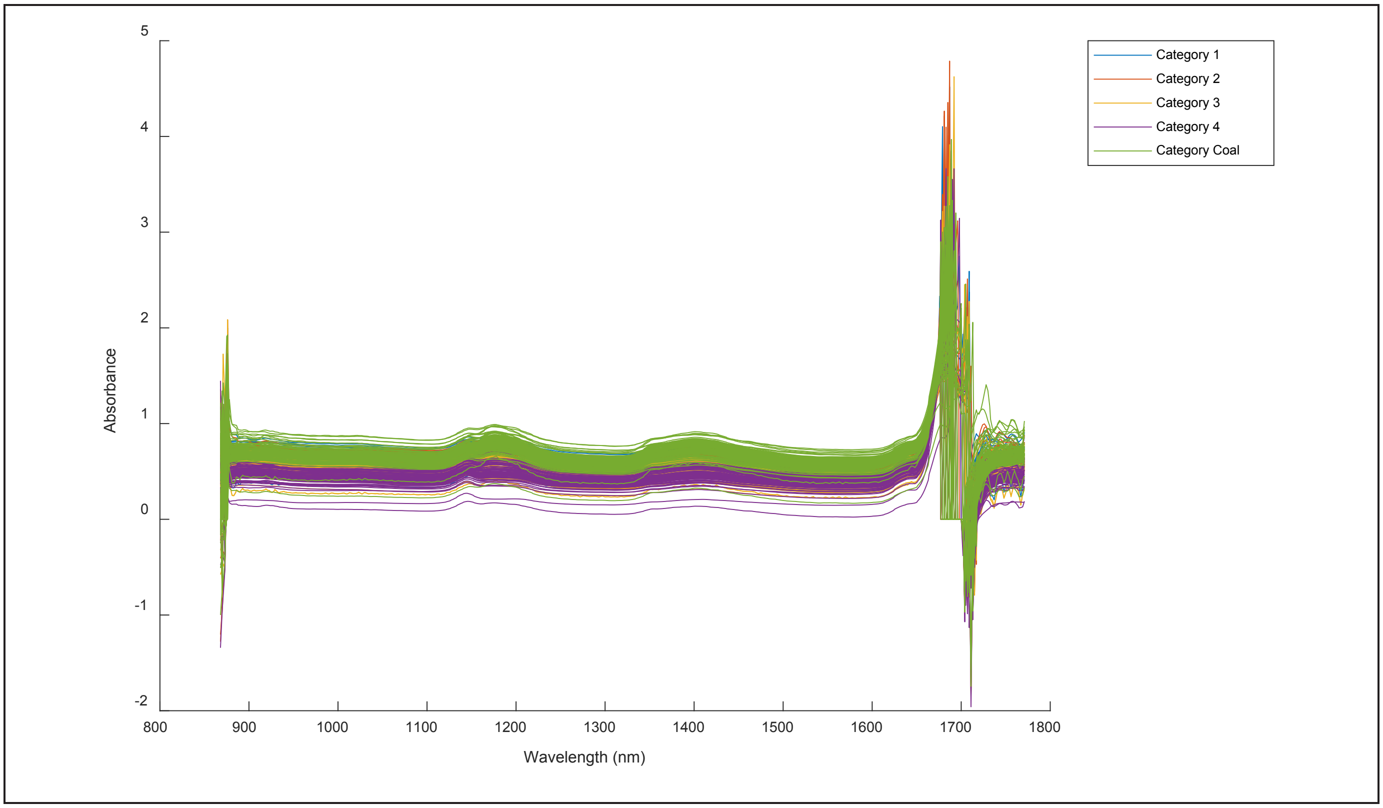

Figure 2. Raw NIR Spectra

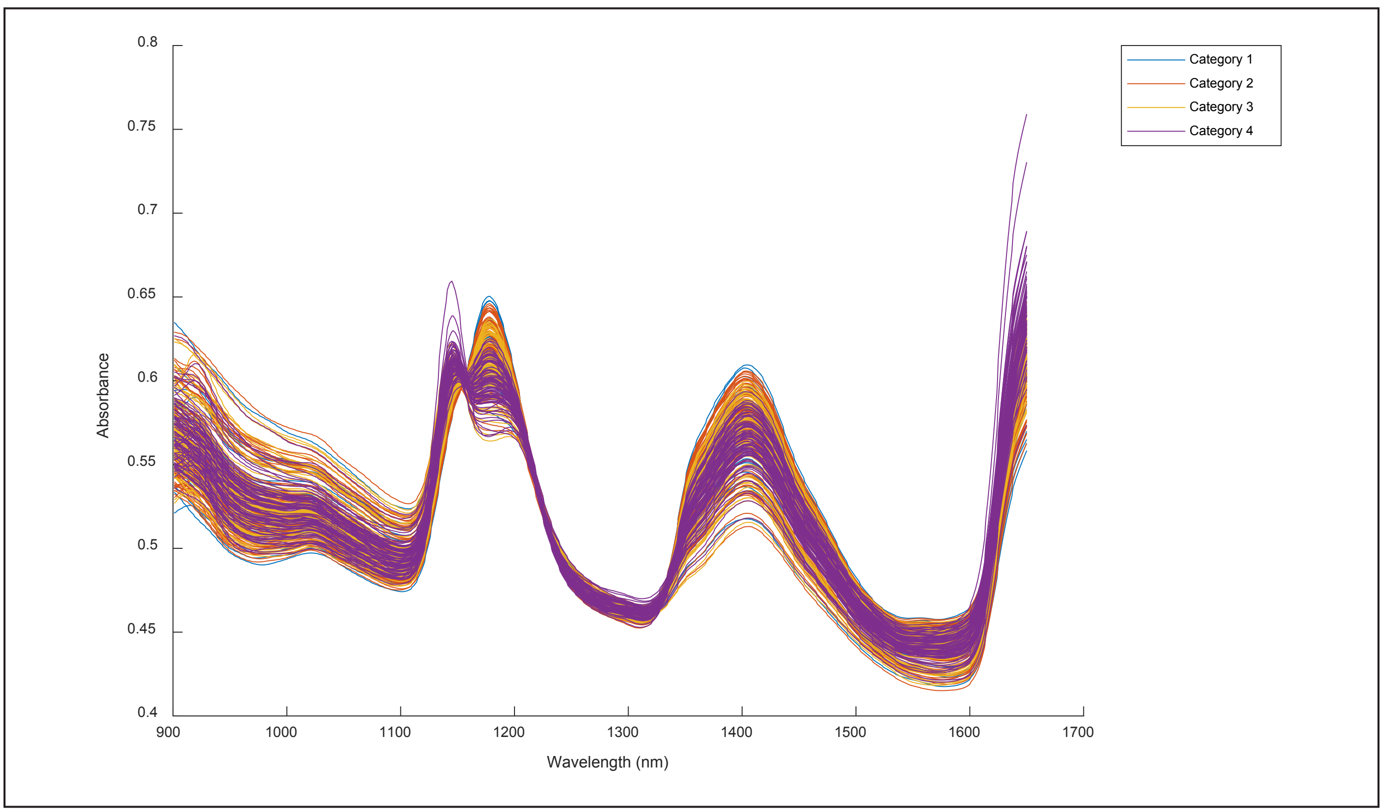

Figure 3. Pre-processed NIR Spectra

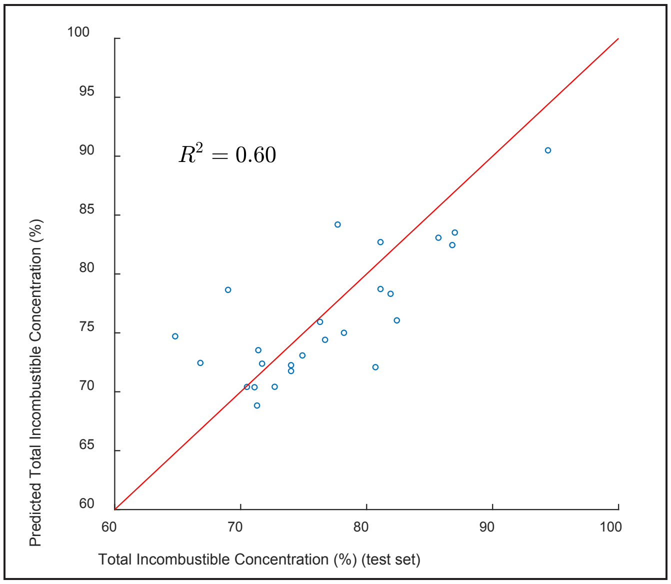

Figure 4. Comparison of Predicted and Calculated Values (Test Set)

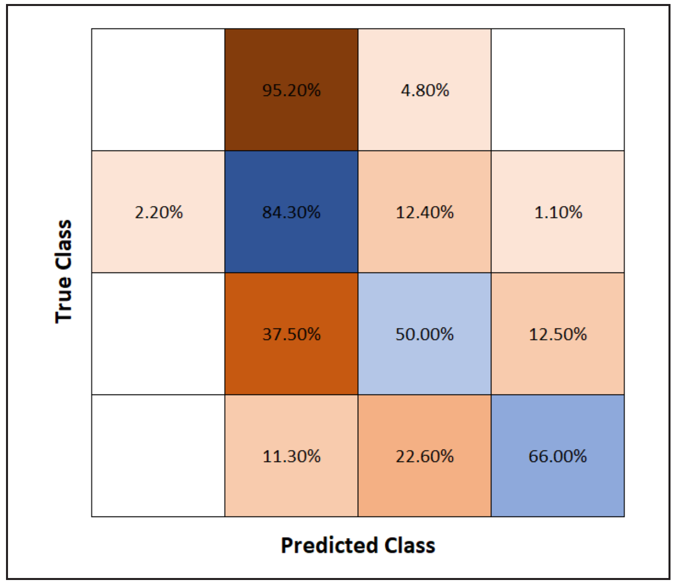

Figure 5. Confusion Matrix for Quadratic SVM Classification Model

suitable regression model for the pre-processed spectra. The analysis concluded that Gaussian Process Regression (GPR) exhibited superior performance compared to other models, and it was fine-tuned with the following hyperparameters: the basic function was set to constant, the Kernel function employed was an isotropic rational quadratic, the Kernel scale was established at 0.024937, sigma was determined to be 51.9962, and the data was standardized. GPR emerged as the optimal choice, demonstrating notable training results, including a Root Mean Square Error (RMSE) of 3.93% and an R2 value of 0.65. As illustrated in Figure 4, the GPR regression model successfully predicted the TIC values for a set of 25 coal-stone dust mixture samples within the test set. The evaluation yielded notable performance metrics with R2 value of 0.60 and RMSE of 4.46%. These results closely aligned with the performance metrics obtained during the training phase using the train set. Such close correspondence between training and test results indicates that the model achieved a balance between accuracy and generalization, suggesting that it did not suffer from overfitting and demonstrated stability in its predictive performance. This outcome underscores the robustness and reliability of the GPR regression model in capturing the underlying patterns in the data.

Classification Models

The analysis of classification models included Decision Tree, Support Vector Machine (SVM), Ensemble and Neural Network (NN) classifiers. It was determined that the Ensemble classifier displayed the most robust performance compared to the other models under consideration. It was further optimized with the following hyperparameters: employing the AdaBoost ensemble method, a maximum of 8 splits, 10 learners, and a learning rate set at 0.53538. The Ensemble classifier emerged as the preferred choice, showcasing notable training results, which included an accuracy rate of 62.6%. The corresponding confusion matrix is illustrated in Figure 5.

The Ensemble classifier underwent further evaluation process using an independent test set to assess the classifier's predictive performance and its ability to generalize to previously unseen data. As shown in Figure 6, the classifier was employed to predict the categories of 25 coal/stone dust samples within the test set, resulting in an overall accuracy rate of 56%. It's worth noting that this accuracy value deviates from the performance observed during the training phase with the train set. This discrepancy can be attributed to the specific challenges encountered by the Ensemble classifier, particularly in accurately classifying Category 1 (TIC < 70%) samples. Despite this variance, it is important to recognize that the classifier's performance aligns with expectations, given the complexities associated with Category 1 classification. In comparison, the classification model demonstrated a high accuracy of 76.92% for Category 2 (TIC = 70%–80%).

Regression Versus Classification Models

Two distinct models were successfully developed based on the machine learning technique: regression and classification. The regression model yielded promising results,

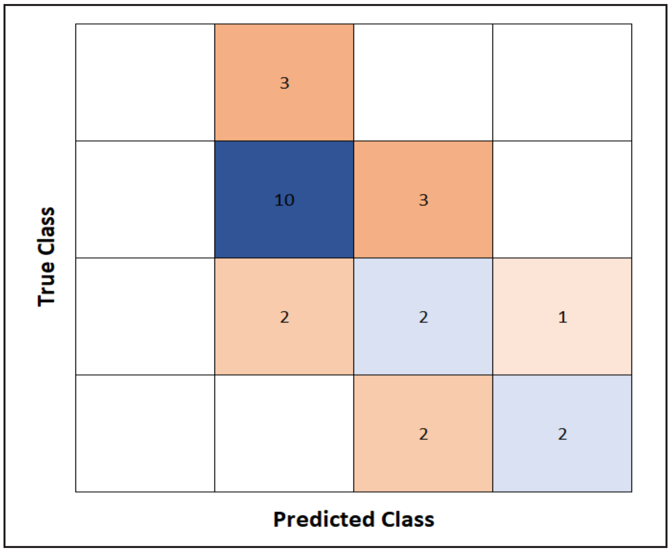

Figure 6. Confusion Matrix for NIR Classification Model (Test Set)

achieving a Root Mean Square Error (RMSE) of 4.46%. The classification model, on the other hand, demonstrated impressive accuracy, reaching 76.92% for Category 2 (TIC = 70%–80%). Nevertheless, the overall accuracy of the classification model stands at 56%, which is primarily attributed to challenges encountered by the classifier in accurately categorizing instances within Category 1 (TIC < 70%).

CONCLUSIONS

Two models, regression, and classification, were evaluated for the data acquired using Stellarnet NIR ADK portable spectrometer. The regression model achieved a RMSE of 4.46% and accuracy of R2 equal to 0.60. The classification model demonstrated a high accuracy of 76.92% for Category 2 (TIC = 70%–80%), however, its overall accuracy of 56% requires further analysis with the main difficulty encountered during the classification within the grouping of Category 1 (TIC < 70%).

FUTURE DEVELOPMENTS

Further refinement and optimization of the models for Stellarnet NIR ADK are in progress including:

1. Refinement of spectra correction techniques,
2. Optimization of smoothing methodologies, and
3. Identification of machine learning algorithms best suited to the spectral data.

ACKNOWLEDGMENT

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24-026

Development of a Comprehensive Mine Plan Approach for the Extraction of Icy Regolith on the South Pole of the Moon Using Surface Mine Modelling Software

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One of the first activities after returning to the Moon will be finding sources of water and materials for the construction of human settlements and other infrastructure. There is evidence of the existence of deposits in the bottom of craters at the South Polar region and in flat areas around. Based on geological data from the Moon, a block model representing a deposit or icy regolith has been defined in the vicinities of Shackleton Crater, with unique characteristics of shape, thickness, and water contents. A mine plan utilizing surface mine modeling software for ore extraction from an open pit- type of excavation to a delivery point near a water processing facility is proposed, with monthly, quarterly, and yearly schedules. Production results, dashboard charts and progress of the topographic changes are also presented.

INTRODUCTION

From all the things to do when arriving on the Moon, humans must find sources of icy regolith and start sampling for the definition of ore bodies and reserve estimation. As opposed to the Earth, where the target are base metals or non-metal minerals, the one of the most important is finding the areas where there is abundance of water sources, and raw materials for construction. The areas with more probability to find these resources are the Permanently Shadowed Regions at the South Pole (Figure 1).

Figure 1. The Moon South Pole and Shackleton Crater (source: Moon Trek)

In such locations, there is the presence of water mixed with the regolith, accumulated over millions of years as a result of comets passing sufficiently close to the Moon and the accumulated water ice not being able to evaporate due to the almost null exposition to the Sun. Discoveries such as these, have opened the immense opportunity to consider the extraction of this water to be decomposed into oxygen and hydrogen, while additionally finding adequate processes to extract other valuable minerals such as base metals, precious metals and Rare Earths.

With the use of Moon Trek, a public domain geographical tools, it is possible to have an enhanced view of these regions, using data from the Lunar Reconnaissance Orbiter (LRO), which has mapped the entire South Pole, removing the shadows. We can now appreciate the bottom