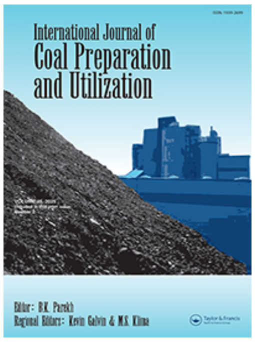

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Prediction of HGI of South African coalfields: a comparative application of ANN, SVR and LSTM models

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ABSTRACT
Hardgrove grindability index (HGI) is a significant index used to determine a mill's capability and overall efficiency in the grinding of coal. There are several factors that affect HGI due to the complex nature of coal. The influence of proximate analysis, calorific value, total sulfur, and pyrite content on the HGI values of 292 coal samples from South African coalfields were examined. Predictive models of HGI are developed by using soft computing techniques such as Long Short-Term Memory (LSTM), support vector regression (SVR), and Artificial Neural Network (ANN). This study shows that ANN is the most effective predictive model for all the three coalfields, with SVR models being second and LSTM models being the least effective. The correlation between the predicted value and the input data is established by using the cosine amplitude method (CAM). It was found that HGI is most influenced by the fixed carbon content, calorific value, ash content and volatile matter content while pyrite has the least influence.

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KEYWORDS
Hardgrove grindability index; machine learning; coalfields; coal properties

Introduction

The practical implications of grinding coal into a fine powder and using it as a pulverized fuel are significant. The overall efficiency of the mill and power plant can be improved if coal can be grinded easily, as grinding is a laborious process that requires energy. The grindability of coal depends on its rank and inherent mineral content, which are related to its maceral group composition. To estimate coal grindability, a method called the Hardgrove grindability index (HGI) (ASTM D409–51) is used. The HGI provides an insight into the behavior of coal, the ease of grinding coals, and the power required for grinding coals in a pulverizer/mill. There are other techniques to estimate the grindability of coals, but HGI is the most frequently employed (Speight 2005).

The entire coal value chain, from mining to processing and utilization, is affected by coal grindability. It influences the economics, capabilities, and efficiency of the comminution equipment both in the processing plants and the power plants (Wang et al. 2018). According to Tymoszuk et al. (2019), the grindability of coal has a direct impact on the

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performance of the mill in a power plant. In addition, reducing the size of coal consumes roughly 5% of the energy produced in most coal-fired power plants (Doroodchi, Zulfiqar, and Moghtaderi 2013). This value varies from one coal to another, as the hardness, fracture resistance, and tenacity of coal depend on its organic and inorganic components, which vary from one coalfield to another (Rubiera et al. 1999; Ural and Akyıldız 2004). The blending of coal, which is a common practice among coal traders, also contributed to this phenomenon. This increases the expense of maintaining the milling parts, as the blending is mostly done based on the physiochemical properties of the coal, not based on the grindability of individual coals in the blend. The inorganic mineral composition of coal, such as quartz and pyrite, tends to abrade the steel of the milling portion, which in turn impairs the mill's efficiency (Nahvi, Shipway, and McCartney 2009). The HGI of coal is also influenced by the high ash content, low volatile matter, and high moisture content, as reported by Falcon and Falcon (1987). According to the same authors, the moisture content of low rank coals appears to have an impact on its grindability but with no influence on higher rank coals. It is therefore important to determine the composition of these coals and most importantly, the HGI value of the coal prior to application. This study offers a predictive method as a viable alternative to the HGI method, which has been found to be laborious, time-consuming, and costly (Deniz and Umucu 2013).

The use of computer-developed tools like generalized regression neutral network (GRNN) and non-linear multivariable regression (MLR) in correlation with the proximate data from coal have been used to produce linear relationship with HGI. Based on this as well as the correlation with petrographic results, the HGI of coals can be predicted. Bagherieh et al. (2008) developed an artificial neutron network (ANN) that combines petrographic data to forecast coal HGI. The result shows that the inorganic mineral composition in coal influences the HGI of coals. A strong correlation was also established between the proximate analysis and the grindability of coal, leading to Statistical Grindability Index (SGI) (Sengupta 2002). Peisheng et al. (2005) also developed a model based on coal proximate data to predict the HGI using a Generalized Regression Neural Network (GRNN). Venkoba-Rao and Gopalakrishna (2009) also used a support vector regression (SVR) model based on proximate analysis to predict the HGI of coal. The coal calorific value, combined with the proximate and ultimate data, was used to predict HGI, based on Artificial Neural Network (ANN) (Khoshjavan and Rezai 2013). Another investigation by (Bagherieh et al. 2008) led to a model with a maximum R^2 coefficient of 0.92 being developed after integrating petrographic analysis data with proximate and ultimate analyzes. Chelgani et al. (2008) produced three prediction models of HGI using the least-square regression approach. Additionally, the authors used Feed-forward Artificial Neural Networks (FANN) to enhance the predictions, with R^2 coefficients of 0.89, 0.89, and 0.95, respectively, achieved. Another study from Matin et al. (2016), incorporating analyzes of proximate, ultimate, and petrographic creates a good model for predicting HGI. The findings presented were positive, but there is still a need to enhance the performance of the models reported to reach R^2 values above 0.95.

In this study, the comparative performances of (LSTM), support vector regression (SVR) and back-propagation neural network (BPNN) were used to develop predictive models for HGI. The use of these models to predict HGI for coal from different coalfields has not yet been established in the literature. As coal will remain part of our energy source into the future, there is still a need for more research and the application of innovative approaches that could lead to its efficient comminution, processing, and use. In addition, the fact that coal from different coalfields has different grinding characteristics necessitates the need for this study. The impact of coal blending on its grindability has been the subject of numerous studies (Ananda-Babu, Lawrence, and Sivashanmugam 2018; Idris et al. 2019; Miroshnichenko et al. 2019). Findings have shown that coal blends of different ranks or types possess a variety of varied and unpredictable HGI values (Idris et al. 2019). Experimentally, emphasis is laid more on the HGI of the final coal blend than on the individual coals from different coalfields. By using a mathematical model created for these coalfields, both the HGI of the individual and the final blend can be obtained simultaneously, given that the model's input parameters are additive.

The aim of this study is to develop a predictive model of HGI based on soft computing techniques that satisfies the criteria linked to the raised concerns. Direct evaluation of how different input features affect the model's output is difficult with complex machine learning algorithms. However, in this study a sensitivity analysis [cosine amplitude method (CAM)] was adopted. This could automatically assess the influence of each input parameter on the predicted value.

Research Methods

Sample Location

A total of 292 coal samples were collected from different coalfields in South Africa for this study. On the Witbank coalfield, which encompasses Middleburg and Secunda, 147 coal samples were taken. In KwaZulu Natal coalfields (Vryheid, Utrecht, and Ulundi), 89 samples were taken, and 56 from the Ermelo coalfield (Belfast – Carolina). These coals differ (have distinct organic constituents and mineral matter) and are less mature than carboniferous coal found in the northern hemisphere.

Sample Preparation and Testing

The collected coal samples were bagged and labeled for analysis and storage. The coals were thereafter subjected to different physiochemical analyzes and mechanical testing. The proximate analysis was conducted in accordance with the (ISO 11722 2013) for the inherent moisture content (%) (ISO 1171 2010), for the ash content (%) (ISO 562 2010), for the volatile matter content (%), with fixed carbon calculated by difference. The ultimate and total sulfur analysis of the coal was carried out in compliance with (ASTM, D5373–14, 5373–14) and (ISO 19579 2006). For the CHN, a LECO CHN 628 was utilized, and approximately 0.25 g of the coal was used for the analyzes at a temperature up to 1450°C. The calorific value was determined in accordance with ASTM D5865–04. The HGI analysis was conducted in accordance with the (ISO 5074 2015) on a 50-gram coal sample in a grinding unit which rotates at a speed of 60 rev/sec. The product coal obtained after grinding is then sieved to pass through −75 μm screen. The data from the HGI provided information regarding the relative ease and power required for grinding coals in a pulveriser/mill.

Predictive Models for HGI

Coal is a complex material with a range of properties, and the interactions between coal properties are extremely complex. The HGI values of coals investigated varies within the coalfields examined. This necessitates establishing predictive models based on proximate analysis, calorific value, total sulfur, and pyrite contents to predict the HGI of coals. Various soft computing models (ANN, SVR and LSTM) were developed to predict the HGI of coals from selected South African Coalfields by using the experimental data obtained in the laboratory. For a fair comparison, the same randomly divided train, test, and validation datasets were used to train, test, and validate all these techniques.

Descriptive Statistics of the Experimental Parameters for the Coalfields

Table 1 to 3 provides a summary of all the statistical features of the sample from the Witbank, Ermelo, and KwaZulu Natal coalfields, respectively. The normality test was carried out on the datasets before model development by using the Shapiro–Wilk normality test. The obtained parameters for the Witbank coals rejected normality at a 5% decision level, except for the volatile matter, as shown in Table 1. For the samples from the Ermelo coalfield,the obtained experimental datasets rejected the normality at a 5% decision level, except for total sulfur, which accepted the normality as shown in Table 2. For the KwaZulu Natal coals, all the experimental results rejected the normality except for the calorific value at 5% decision level as shown in Table 3. All the normality obtained are also supported by the skewness and Kurtosis values presented in the Tables 1 to 3. The statistical description/test revealed that the investigated properties are complex and simple regression model may not be

Table 1. Descriptive statistics for the Witbank coalfield.

Model parameter	N total	Mean	Std	Sk	Kurt	Min	Median	Max	p-value	Decision at level (5%)
CV	147	26.92	2.16	−0.65	0.18	19.5	27.5	31.2	4.13E−04	RN
M	147	3.37	1.18	0.85	0.35	1.9	3.1	7.6	4.00E−07	RN
A	147	14.72	4.38	0.84	1.30	6.6	14	32.4	3.58E−04	RN
VM	147	26.33	2.76	0.28	−0.19	20.1	26	33.1	0.12653	CRN
FC	147	55.58	3.57	−0.36	0.38	42.1	55.2	61.9	0.00645	RN
TS	147	0.70	0.40	2.12	6.81	0.21	0.59	2.87	4.11E−12	RN
Pyrite	147	0.82	0.69	2.17	6.26	0.06	0.65	4.28	3.85E−13	RN
HGI	147	54.96	5.71	0.87	1.39	43	54	76	4.15E−05	RN

*RN-reject normality; CRN-can't reject normality; CV: Calorific value; M: Moisture content: A: Ash content: VM: Volatile matter: FC: Fixed carbon: TS: Total sulfur.

Table 2. Descriptive statistics for the Ermelo coalfield.

Model parameter	N total	Mean	Std	Sk	Kurt	Min	Median	Max	p-value	Decision at level (5%)
CV	56	25.84	2.10	−0.71	0.02	20.4	26.3	29.3	0.0064	RN
M	56	3.87	1.09	−0.41	−0.66	1.7	4.05	5.8	0.02263	RN
A	56	17.02	4.28	0.83	0.33	9.2	15.7	28.6	0.00473	RN
VM	56	23.74	6.35	−0.99	0.92	7.7	24.3	34.5	2.65E−04	RN
FC	56	55.37	6.06	1.63	2.67	45.8	54.1	74.7	2.08E−06	RN
TS	56	0.73	0.33	0.23	−0.44	0.15	0.75	1.54	0.44197	CNR
Pyrite	56	0.76	0.49	0.92	0.84	0.06	0.67	2.23	0.00551	RN
HGI	56	57.30	8.74	0.40	−0.32	40	57	78	0.36611	CNR

Table 3. Descriptive statistics for the KwaZulu coalfield.

Model parameter	N total	Mean	Std	Sk	Kurt	Min	Median	Max	p-value	Decision at level (5%)
CV	89	29.80	1.53	−0.23	−0.35	26.2	29.9	33.2	0.5941	CNR
M	89	1.82	0.52	0.90	1.99	0.9	1.8	3.9	0.00312	NR
A	89	13.39	3.44	0.79	1.50	5.9	13.1	23.8	0.00223	NR
VM	89	12.58	6.51	1.13	0.22	5.2	9.6	30.3	4.70E−08	RN
FC	89	72.20	7.87	−0.80	−0.48	55.3	74.9	84.5	2.19E−06	RN
TS	89	1.11	0.64	2.83	9.82	0.44	0.98	4.26	5.89E−12	RN
Pyrite	89	0.95	1.05	3.58	14.29	0.11	0.71	6.47	1.60E−14	RN
HGI	89	54.28	13.95	0.52	−0.69	33	52	85	4.41E−04	RN

able to capture the disparities in the model parameters. Therefore, we proposed AI based models for the reliable predictions of the HGI of coal from these different coalfields.

Development of Predictive Models for HGI Using Machine Learning Techniques

Artificial Neural Network (ANN)

The feed-forward ANN model with back propagation training algorithm is proposed for predicting the grindability index of the coals used in this study. The ANN is in layers with input layer i.e. the model parameters, while the hidden layer manipulates the parameters with the aid of transfer function to emulate the presented targeted output in the output layer. The number of input layer neuron is proportional to the number of model independent parameters, the hidden layer neurons are usually obtained by trial-and-error approach. The number of neurons in the output layer is also proportional to the number of targeted output parameters. The proposed ANN model in this study was implemented in the MATLAB environment with just three layers. The datasets were divide into three in the ratio 0.7:0.15:0.15 for the respective training, testing and validation cases after the data normalization. The input layer has 8 neurons and the output layer has 1 neuron. The hidden layer neurons were varied between 2 and 20. About 49 models were tried for all the three coalfields (19 per coalfield). The Levenberg-Marquardt training was used with the back propagation training algorithm and tan sigmoid transfer function was used at the hidden and output layers. Each models are evaluated using the coefficient of correlation (R) index and the model that has the best *R* values in the three phases is selected for each of the three coalfields.

Long Short-Term Memory (LSTM)

The LSTM is an advanced Recurrent Neural Network (RNN) as it eliminates the vanishing gradient problem in the traditional RNN network by neglecting the redundant information in the network. LSTM has three significant steps which involves training of the model to forget the irrelevant information/data. The second step requires the learning of the data and the last step returns the updated data from the incumbent-time step to the later-time step. The LSTM was employed to predict the grindability index of coals used in this study. The LSTM parameters used in implementing the models in MATLAB are shown in Table 4. The same number and kind of datasets used in training, testing and validation of ANN models are also used for the LSTM model.

Table 4. LSTM parameters.

Parameters	Description
Solver	Adam
Hidden unit number	100
Epoch	3000
Gradient threshold	0.01
Initial learning rate	0.0001

Support Vector Regression (SVR)

The support vector machine for regression is implemented in Weka software to predict the HGI of coals by using the SMO algorithm proposed by Shevade et al. (1999). This was used with default RegOptimizer. The polykernel function of order 2 was used with complexity parameters varying between 1 and 4. The increase in the order of the polykernel and the complexity parameters does not make any improvement on the obtained results. The performances of 12 different models (i.e. 4 models per each of the coalfields) are presented in the next section.

Results and Discussion

ANN

The performances of different ANN models (ANN7-2-1 to ANN7-20-1) tried based on the R values are presented in Figs. 1–3 for the respective Witbank, Ermelo and KwaZulu Natal coalfields. For the Witbank coalfield, ANN7-16-1 has the best performance for the training, testing and validation phases as all the predicted data points for the model between spider lines 0.98 and 1 (Fig. 1). For the Ermelo coalfield, the performances of the models are generally good at both the training, testing and validation cases except the models ANN7-2-1 and ANN7-3-1. The optimum ANN model for this Ermelo coalfield is ANN7-12-1 (Fig. 2) with its R values for the training, testing and validation cases lying almost on the circumference of the spider plot. For the KwaZulu Natal coalfield, most of the simulated ANN models have a promising R values, but the model ANN7-14-1 (Fig. 3) gives the optimum R values for the training, testing and validation phases. For each of the locations, the overall performances of each of the models were visualized together with the plots of the predicted and measured values against the nominal data points. The linear fitting of the measured and the predicted HGI for each of the cases is also associated with + or −3% error bars. The results revealed that the predictions of each of the selected optimum ANN networks are close to the actual predicted values most importantly the Ermelo coalfield while all the data points fall within the error bars. Similar observation is observed in the KwaZulu Natal coalfield except that a point glaringly falls outside the error bars. While in the Witbank coalfield, some of the points fall outside the error bars. Nevertheless, the models give reliable predictions of the HGI of coal.

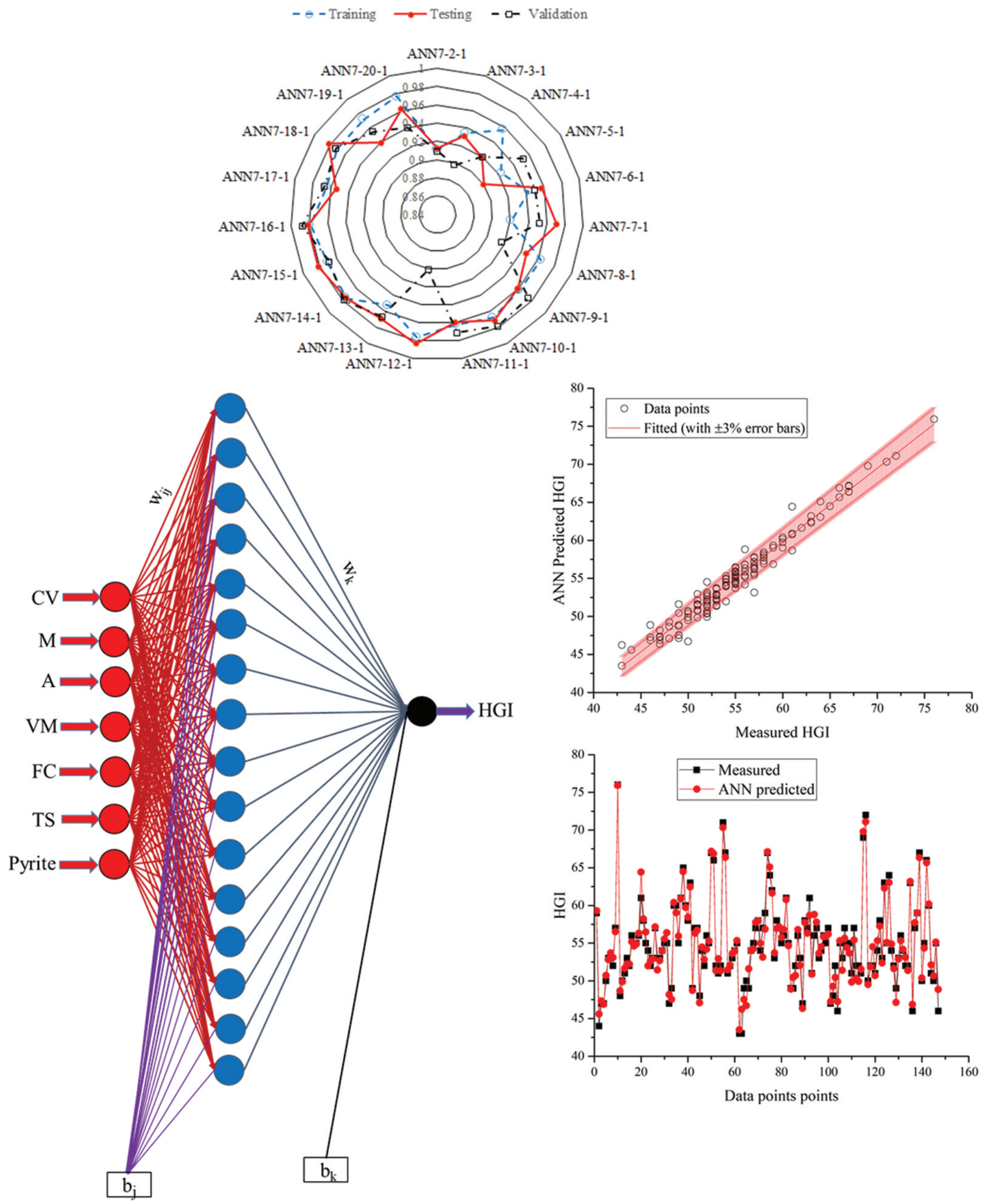

Figure 1. Obtained results using ANN for Witbank coalfield.

SVR Model

This study also used various SVR models to predict the HGI of coals under investigation. The complexity parameter C was varied between 1 and 4 for each of the models (Figs. 4–6). For the Witbank coalfield, the C4 that implies the complexity parameter of 4 is favored while for the Ermelo coalfield, the complexity parameter C2 is favored and for KwaZulu

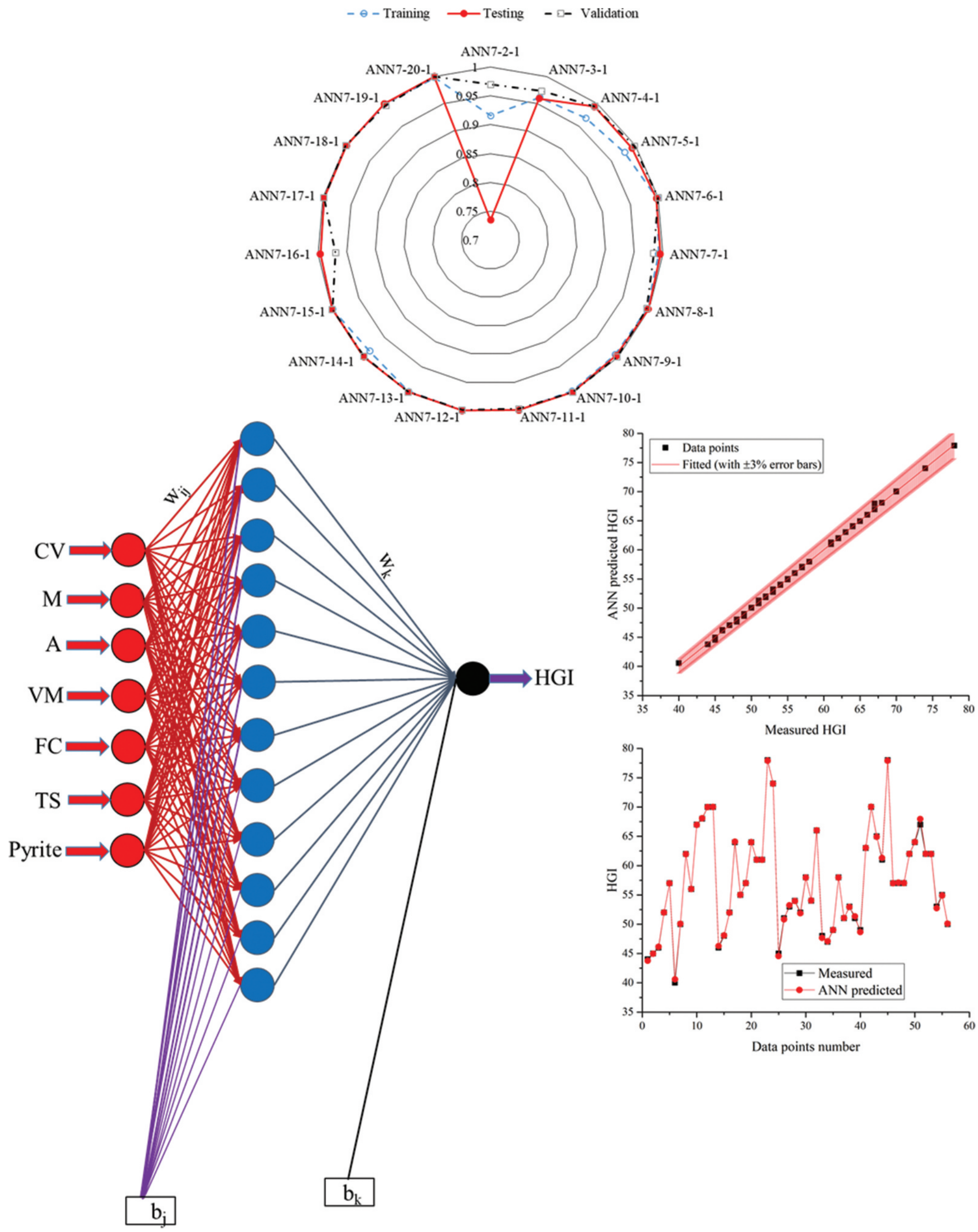

Figure 2. Obtained results using ANN for Ermelo coalfield.

Natal coalfield, C1 is favored. The number shown in the spider plots are the R values. The linear fitting of each of the predicted values are also associated with the + or −3% error bars. The results reveal that majority of the data points fall outside the error bars for the three coalfields investigated. The more data points are scattered outside the error bars, the lower the expected correlation between the measured and data points. This is revealed by the

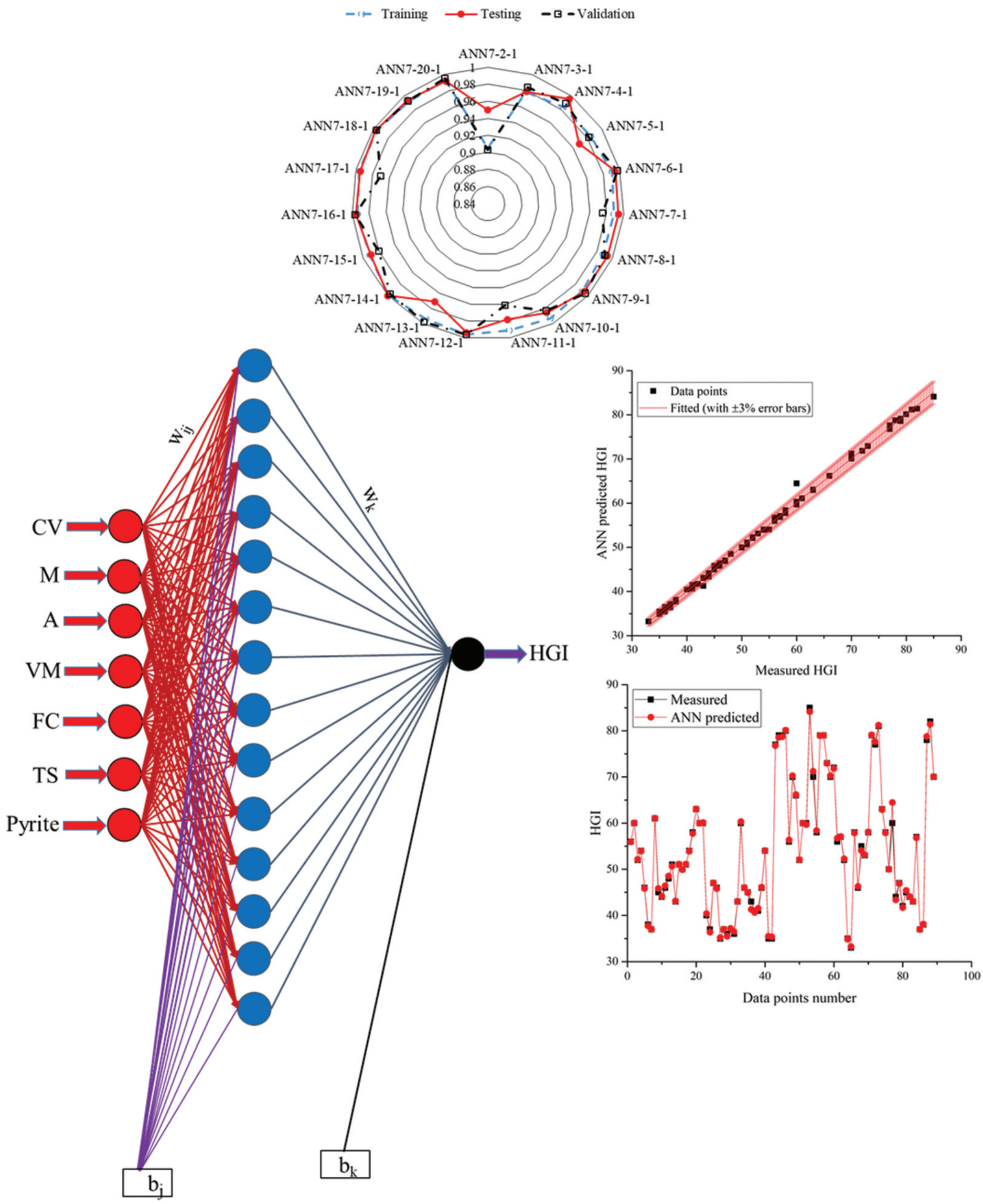

Figure 3. Obtained results using ANN for KwaZulu Natal coalfield.

measured and predicted HGI against the data points on the right side of the fitted figures (Figs. 4–6). This consequently implies the low performance indicator such as R value.

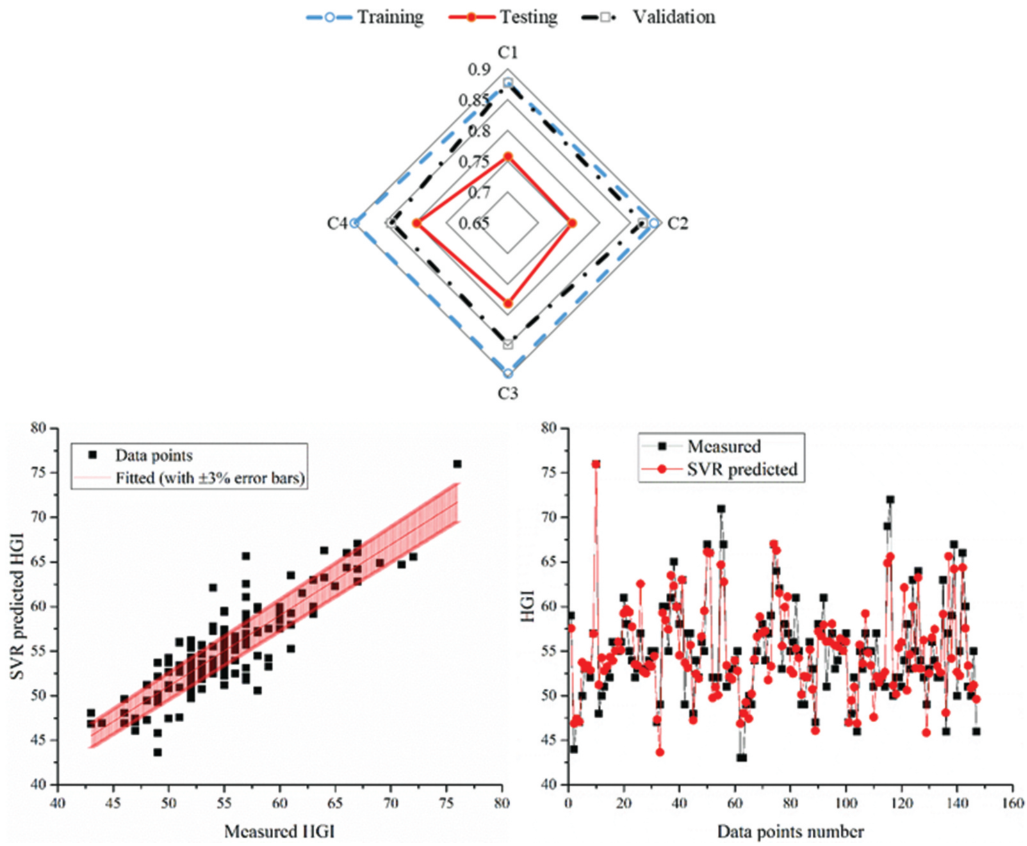

Figure 4. Obtained results using SVR for Witbank coalfield.

LSTM

The purpose of using the LSTM is to propose a more advanced model that can capture the inherent complexity in the coal samples, as revealed in the statistical analysis conducted in section 3. The results obtained using the LSTM parameters are presented in Table 4. The observed performances of the LSTM model for the training, testing, and validating cases using the same set of parameters as those used in the ANN and SVR cases are shown in Figs. 7–9. Generally, for all the three cases, the performances of the testing phases are poor, most specifically for the coal samples from the KwaZulu Natal coalfield. The performance of the validation phase of the samples is also low, except for those from Ermelo and Witbank coalfields. The LSTM performances is low for the cases considered in this article.

Model Selection Using ANOVA

The ANOVA analysis was used to select the best machine learning models among the proposed models for the prediction of HGI of coals used in this study, similar to the approach by Lawal et al. (2023). For this study, the overall datasets used in developing the models are used in this selection. The ANOVA results obtained for each of the three coalfields are presented in Tables 5–7. The higher the F value, known as the ANOVA

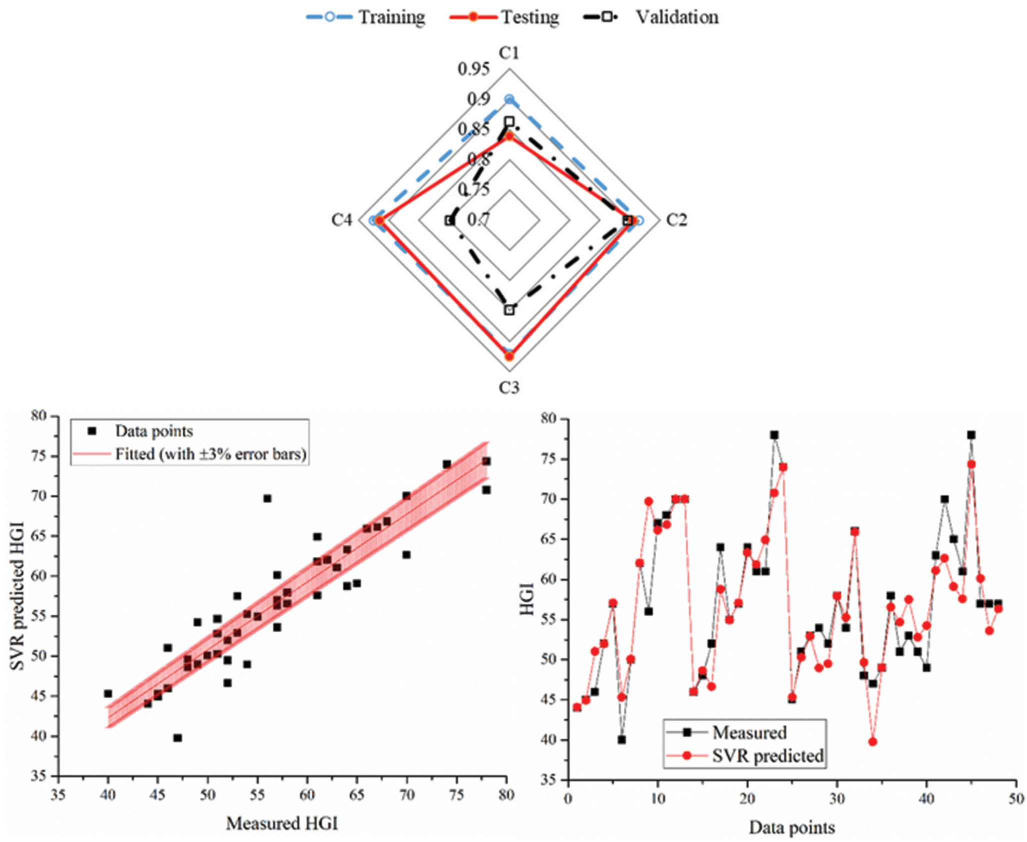

Figure 5. Obtained results using SVR for Ermelo coalfield.

coefficient, the better the model performance because it implies a low mean square error sum. Hence, based on the ANOVA analysis, the F-values of the ANN models for the Witbank, Ermelo and KwaZulu Natal coalfields are 3626.9, 100916.8 and 45,215.9 while for the SVR models, their F-values are 465.9, 200.4 and 914.9 and for the LSTM model, the F-values for the three coalfields are 367.2, 187.5 and 125.1. According to this ANOVA result, the ANN model performs better for the three locations and therefore it is selected to predict the HGI for the three selected locations. This model can be easily expressed in mathematical form using their respective weights and biases. The SVR can also be used most specifically for the KwaZulu Natal coalfield as the F-value obtained for this coalfield is also high. The LSTM seems to be the least suitable model among the models tried in this study.

Sensitivity Analysis

The relative importance of each of the independent model variables are investigated by using CAM as reported by Lawal et al. (2021, 2023), Lawal and Kwon (2023). The relative importance approach has been widely utilized to assess the contributions of the model variables to the model. It is basically the product of the predicted trained output and each model input divided by the square root of the product of their squares. The ANN model's

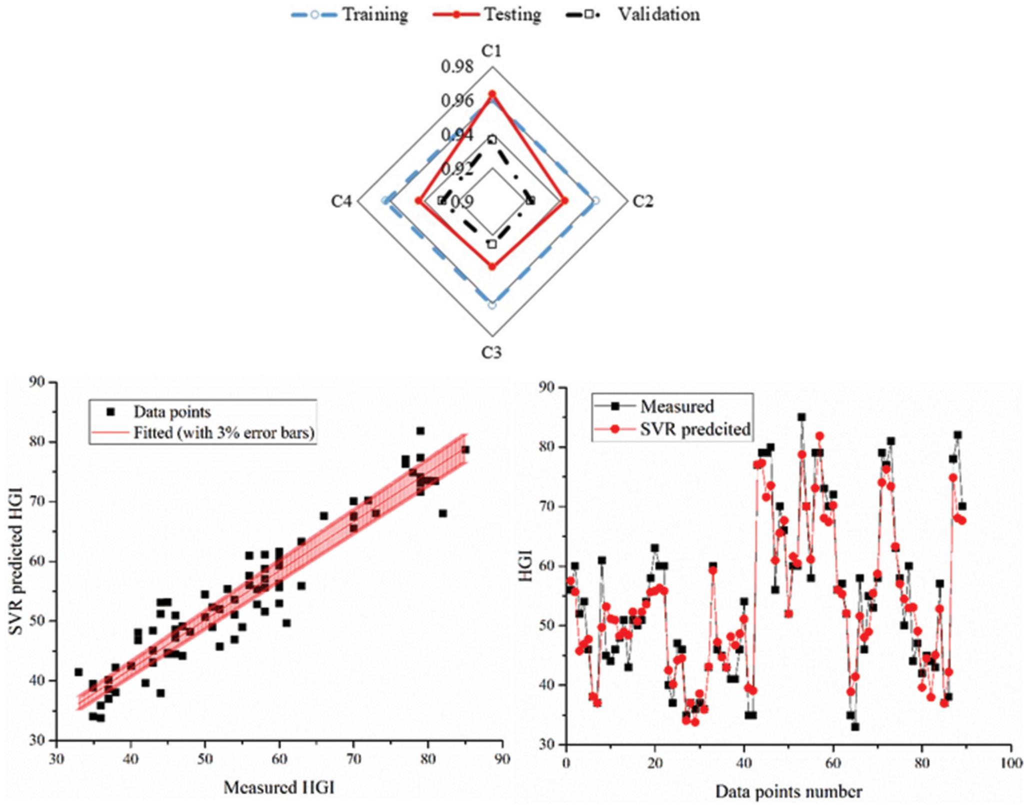

Figure 6. Obtained results using SVR for KwaZulu Natal coalfield.

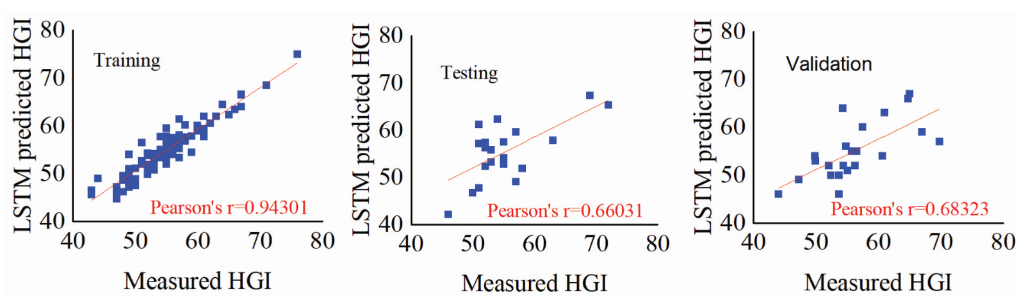

Figure 7. Obtained results using LSTM for Witbank coalfield.

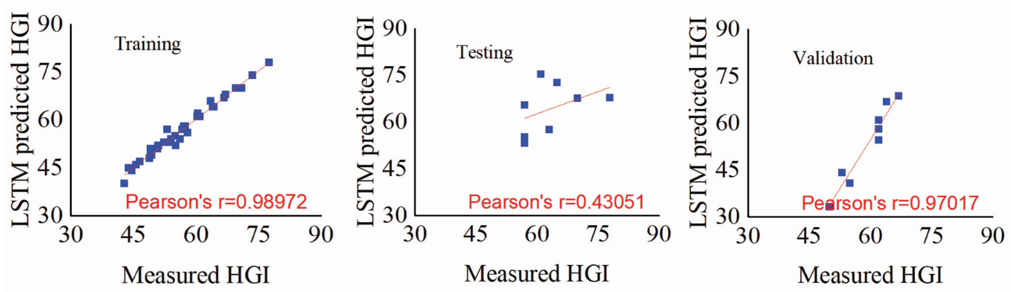

Figure 8. Obtained results using LSTM for Ermelo coalfield.

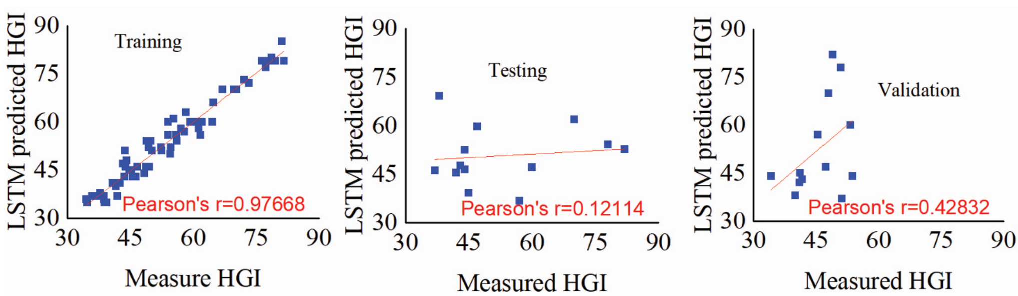

Figure 9. Obtained results using LSTM for KwaZulu Natal coalfield.

Table 5. ANOVA for the ANN models.

	DF	Sum of Squares	Mean Square	F Value	Prob>F
Witbank coalfield					
Model	1	4438.292	4438.292	3626.907	0
Error	145	177.4384	1.22371		
Total	146	4615.73			
Ermelo coalfield					
Model	1	4218.554	4218.554	100916.8	0
Error	54	2.25732	0.0418		
Total	55	4220.812			
KwaZulu Natal coalfield					
Model	1	17149.67	17149.67	45215.87	0
Error	87	32.99774	0.37928		
Total	88	17182.67			

output was utilized for this study due to its outstanding performance. The obtained result is as presented in Fig. 10. The CV, M, A, VM, FC, and TS in Fig. 10 stands for calorific values, moisture content, ash content, volatile matter content, fixed carbon content and total sulfur. For the Witbank coalfield, fixed carbon content, calorific value and volatile matter content are the most influencing parameters. Ash content, fixed carbon content and calorific value are the most influencing parameters for the samples from Ermelo coalfield, while calorific value, ash content and fixed carbon content are the most important parameters in the samples obtained from KwaZulu Natal coalfield. In all the investigated cases, fixed carbon

Table 6. ANOVA for the SVR models.

	DF	Sum of Squares	Mean Square	F Value	Prob>F
Witbank coalfield					
Model	1	3003.333	3003.333	465.8964	0
Error	145	934.7213	6.44635		
Total	146	3938.054			
Ermelo coalfield					
Model	1	2637.048	2637.048	200.3716	0
Error	54	710.6824	13.16078		
Total	55	3347.73			
KwaZulu Natal coalfield					
Model	1	11595.16	11595.16	914.9828	0
Error	87	1102.512	12.67255		
Total	88	12697.68			

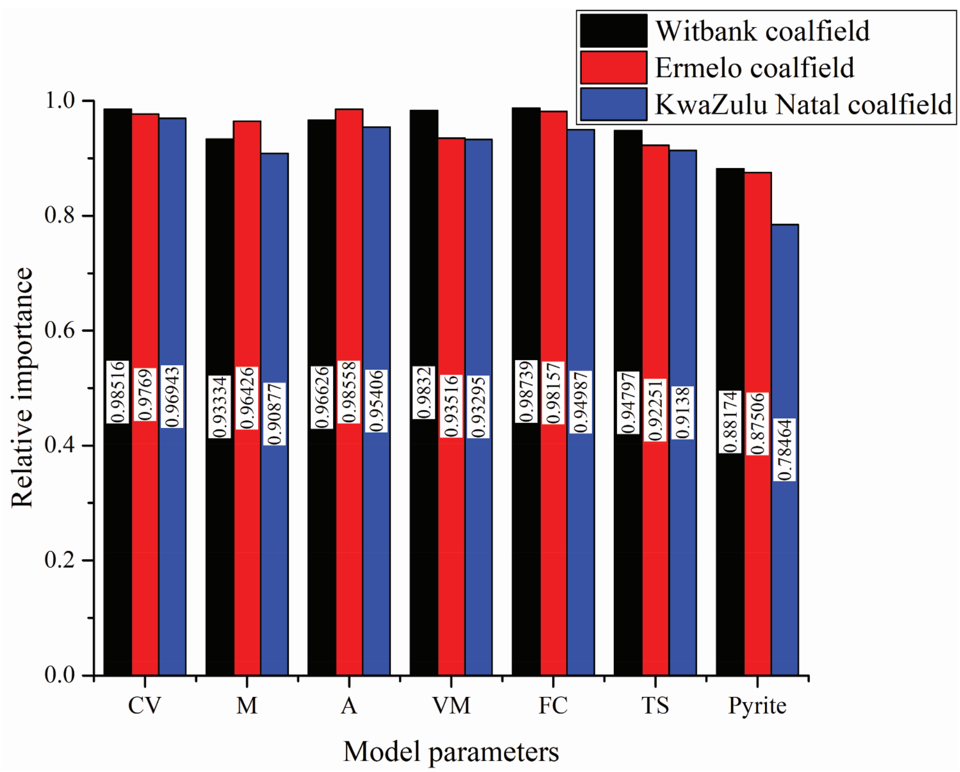

Figure 10. Relative importance of the model independent variables.

Table 7. ANOVA for the LSTM models.

	DF	Sum of Squares	Mean Square	F Value	Prob>F
Witbank coalfield					
Model	1	3152.787	3152.787	367.1686	0
Error	145	1245.08	8.58676		
Total	146	4397.867			
Ermelo coalfield					
Model	1	4040.695	4040.695	187.5473	0
Error	54	1163.427	21.54494		
Total	55	5204.122			
Kwazulu Natal coalfield					
Model	1	7507.15	7507.15	125.0956	0
Error	87	5220.985	60.01132		
Total	88	12728.14			

content, calorific value, ash content, and volatile matter content have a good contribution to the model, while pyrite has the least influence.

Conclusion

Predictive HGI models are established using machine learning methods by incorporating seven parameters (moisture, ash content, volatile matter, fixed carbon, calorific value, total sulfur, and pyrite content) that represent the properties of coals. To explain the relationship between the predicted value and the input data, the CAM approach was adopted. According to this study, the fixed carbon content, calorific value, ash content, and volatile matter had the most significant impact on the HGI prediction, while pyrite had the least impact. The results demonstrate that the LSTM technique was unsatisfactory due to significant disparities between the predicted and actual HGI. However, the ANN technique produced highly accurate predictions of HGI that are more reliable. The finding shows that the model developed is capable of accurate prediction of HGI with a R^2 value of above 0.9. In addition, the study established the viability of ANN and SVR as techniques for predicting and explaining complex correlations between coal properties and HGI of coals from different coalfields.

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No potential conflict of interest was reported by the author(s).

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