Natural Resources Research, Vol. 30, No. 1, February 2021 (© 2020)
https://doi.org/10.1007/s11053-020-09727-y

Original Paper

Rapid Determination of Gross Calorific Value of Coal Using Artificial Neural Network and Particle Swarm Optimization

Hoang Nguyen,[1] Hoang-Bac Bui,[2,3] and Xuan-Nam Bui[4,5,6]

Received 26 April 2020; accepted 25 July 2020
Published online: 11 August 2020

In this study, the gross calorific value (GCV) of coal was accurately and rapidly determined using eight artificial intelligence models based on big data of 2583 observations of coal samples in the Mong Duong underground coal mine (Vietnam). Accordingly, the volatile matter, moisture, and ash were considered as the key variables (inputs) for determining GCV. Seven artificial neural network (ANN) models were developed to estimate GCV as the first stage. Subsequently, the best ANN model (with the highest performance) was selected as the initial ANN model for the optimization process, i.e., ANN 3-12-9-1 model. The particle swarm optimization (PSO) algorithm was applied to perform a global search for the optimal weights/biases of the selected ANN model. This novel procedure is denoted as PSO-ANN. A variety of performance metrics was used to assess the quality of the training process, as well as the models' performance in the testing dataset. The results revealed that the models developed in this study could determine GCV rapidly and accurately. Of those, the PSO-ANN model provided the highest accuracy in estimating GCV of coal with a root-mean-squared error of 182.476, the correlation coefficient of 0.964, the variance accounted for of 96.411, and mean absolute percentage error of 0.016. Besides, the analyzed and compared results also indicated that the PSO algorithm played a significant role in improving the accuracy of the ANN model. It was introduced as an alternative solution to determine the GCV of coal in practical engineering rapidly.

KEY WORDS: Coal, Heating value, Gross calorific value, Energy efficiency, PSO-ANN, Machine learning.

INTRODUCTION

Coal is a sedimentary type of rock formed from traces of ferns and other primitive animals that were covered and buried over millions of years. It is a combustible, black, or dark brown matter (Sivrikaya 2014). It mainly consists of carbon with some other elements, such as hydrogen, sulfur, oxygen, and nitrogen (Bustin et al. 1993; Fagerbakke et al. 1996; Scott 2002; Dong et al. 2011). Many industrial products can be produced from coal, and it is mainly used in thermal power plants, metals, and chemicals (Carraher Jr 2017; Stanger et al. 2018). Nowadays, the global demand for energy is increasing because

[1]Institute of Research and Development, Duy Tan University, Da Nang 550000, Vietnam.
[2]Faculty of Geosciences and Geoengineering, Hanoi University of Mining and Geology, 18 Vien Street, Duc Thang Ward, Bac Tu Liem District, Hanoi 100000, Vietnam.
[3]Center for Excellence in Analysis and Experiment, Hanoi University of Mining and Geology, 18 Vien Street, Duc Thang Ward, Bac Tu Liem District, Hanoi 100000, Vietnam.
[4]Department of Surface Mining, Mining Faculty, Hanoi University of Mining and Geology, Duc Thang, Bac Tu Liem, Hanoi 100000, Vietnam.
[5]Center for Mining, Electro-Mechanical Research, Hanoi University of Mining and Geology, Duc Thang, Bac Tu Liem, Hanoi 100000, Vietnam.
[6]To whom correspondence should be addressed; e-mail: buixuannam@humg.edu.vn

of accelerating industrial development. Thus, coal is considered one of the primary fossil fuels that has a significant role in energy generation, particularly in thermal power plants (Balaeva et al. 2018).

To evaluate the quality of coal as a fuel, gross calorific value (GCV) is considered as an essential indicator (Dung et al. 2020). It has been used in many standards, such as ISO 1928, ASTM D2015, ASTM D3286, CEN/TC 335, and CEN/TS 14918:2005 (Küçükbayrak et al. 1991; Shirazi et al. 1995; Vassilev et al. 2010). To measure GCV, calorimeters have been applied with high accuracies, such as 6200 automatic isoperibol oxygen bomb calorimeter, 6790 detonation calorimeter, 6050 automatic PC bored calorimeter, 1341 plain jacket calorimeter, to name a few. However, these instruments are high-cost, and the operator time per test is $\sim$ 6 min (Parr 2020). Many scientists demonstrated that ash, volatile matter, moisture, fixed carbon, hydro, nitro compounds, oxygen, and sulfur contents have a significant effect on GCV of coal (Andres and Bona 2005; Majumder et al. 2008; Jorjani et al. 2009; Le et al. 2018; Duoc et al. 2020; Yao et al. 2020). They can be easily measured by coal ash volatile matter measuring instruments, near-infrared spectroscopy, or laser-induced breakdown spectroscopy (Posom and Sirisomboon 2017; Lu et al. 2019) with low-cost and high performance with many samples per time. In addition, proximate analysis can also be applied to determine these parameters based on standards. Based on these parameters, GCV can also be relatively calculated by empirical equations (Mason and Gandhi 1983; Given et al. 1986; Balaeva et al. 2018). However, their accuracy is lower than intelligent calorimeters.

To overcome the above drawbacks of the GCV measurement and empirical equations for calculating GCV, many researchers studied and applied artificial intelligence (AI) techniques to estimate the GCV of coal based on the ash, volatile matter, moisture, fixed carbon, hydro, nitro compounds, oxygen, and sulfur contents in coal with promising results. Previous researchers indicated that AI techniques are not only providing high efficiency in terms of energy but also most of the real-life problems (Bui et al. 2019b, 2020a, b; Guo et al. 2019a, b; Nguyen 2019; Nguyen et al. 2019a, b, e, 2020; Nguyen and Bui 2020; Nhu et al. 2020; Tran 2020; Zhang et al. 2020a). Patel et al. (2007) developed several artificial neural network (ANN) models to predict the GCV of coal in India, and they referred to as the robust model for estimating GCV of coal. In another study, Mesroghli et al. (2009) also used ANN and regression analysis for the similar aim of GCV prediction, and they also found a good result therein. Based on AI techniques, Feng et al. (2015) developed and compared the support vector machine (SVM), ANN, and alternating conditional expectation models in estimating GCV of coal. They indicated that the SVM model provided the best performance in determining the GCV of coal. Matin and Chelgani (2016) used another AI technique, i.e., random forest (RF) algorithm, for predicting GCV with satisfactory results. Whereas Hadavandi et al. (2017) found a similar result as those of Feng et al. (2015) when used the SVM model to estimate GCV and investigate its relation to the coal properties. Lu et al. (2017) successfully developed a hybrid AI model to predict the GCV of coal with high accuracy. Accordingly, they developed an ANN model optimized using the genetic algorithm (GA) (i.e., GA-ANN). Additionally, a new hybrid AI model was proposed by Baghban and Ebadi (2019) based on adaptive neuro-fuzzy inference system (ANFIS) and GA, i.e., GA-ANFIS, which generated very accurate predictions. Another hybrid AI model was also developed by Bui et al. (2019a) for predicting GCV, namely PSO-SVR model, and they claimed that the PSO-SVR model can precisely predict GCV with high reliability. In another study, Liu and Lv (2020) applied ANN to calculate GCV of coal, and it has been confirmed that better than empirical formula.

As reviewed above, AI models have been developed to estimate GCV, especially the ANN, ANFIS, and SVR models. However, they do not apply in all areas. Furthermore, novel AI models with the accuracy improved are challenging and the goals of researchers. Therefore, this study proposed a novel hybrid AI model based on a nature-inspired algorithm (i.e., particle swarm optimization (PSO)) and ANN to estimate GCV rapidly, called PSO-ANN model. Whereas previous studies used ANN models (without optimization) or optimized by the GA (i.e., GA-ANN model), the main difference of this study is the use of the PSO algorithm to optimize the ANN model aiming to improve the accuracy of the single ANN model. Herein, seven ANN models were developed to determine the GCV of coal rapidly as the first stage. Then, the best ANN model among seven ANN models developed was selected and further optimized by the PSO algorithm, as the second stage. The obtained results were

then compared and evaluated through performance indices.

STUDY SITE

In this study, the Mong Duong underground coal mine in Vietnam was selected to collect and analyze coal samples. It is located within 106° 36′ 23″ E–106° 36′ 47″ E and 21° 04′ 10″ N–21° 04′ 30″ N in a province of Northern Vietnam (Fig. 1). From a geological perspective, the study site has a complex geological structure that contains several faults and folds (Vite 2017). Stratigraphic studies revealed that the mine comprises 600–800 m of coal-bearing sediments originated from the Hon Gai Formation ($T_{3n\text{-}r}$ *hg*) (Fig. 2). The thickness of coal seams in the mine differs according to location. Coal seams alternate with layers of siltstone, gravel, claystone, and sandstone. The coal in the Mong Duong mine can be classified as anthracite and bituminous coal, which is black, homogeneous, and brittle. In addition, it has a glass or metallic luster and contains black and gray markings. In addition, it has a high calorific value, low sulfur content, and low volatile matter. Therefore, it is mainly used in thermal power plants and industries. Indeed, the rapid determination of the GCV of coal has an essential significance in mining selection, as well as neutralizing coal quality to ensure requirements for thermal power plants and other industries.

DATA COLLECTION AND ANALYSIS

According to previous researchers, GCV of coal can be affected by ash, volatiles, moisture, fixed carbon, water, nitro compounds, oxygen, and sulfur content (Wu et al. 2017; Gómez et al. 2018; Musa et al. 2018; Bhatt et al. 2019; Zhang et al. 2020b). However, many researchers claimed and recommended that ash, moisture content, volatile matter, and fixed carbon should be used to estimate GCV of coal (Matin and Chelgani 2016; Wen et al. 2017; Begum et al. 2019; Onifade et al. 2019). Therefore, ash, moisture content, volatile matter, and fixed carbon were taken into account as the influential parameters that can be used to estimate GCV of coal. Considering the fixed carbon, it was determined based on the ASTM method D2013 or ASTM practice D346. Accordingly, fixed carbon can be calculated by the following equation:

$$\text{Fixed carbon} = 100 - [(\text{Moisture}) + (\text{Volatile}) + (\text{Ash})],\ \% \quad (1)$$

From the statistical point of view, it is clear that the fixed carbon, moisture, volatile, and ash have a high correlation based on Eq. 1. Therefore, fixed carbon should be removed to ensure the accuracy of the predictive model. Finally, only moisture (M), volatile matter (VM), and ash (A) are used to estimate GCV of coal in this study.

For data collection, 2583 coal samples from different coal seams in the Mong Duong underground coal mine were collected and analyzed (Vite 2017). GCV was determined by the Bomb calorimeter (Model Parr 6200) based on the ASTM standard (D5865-04). The input parameters (i.e., M, VM, and A) were determined by proximate analysis based on the ASTM standard (D3172). Some of the samples, as well as the distribution of the GCV dataset used, are illustrated in Table 1 and Figure 3.

PRINCIPLE OF THE AI METHODS USED

Artificial Neural Network

ANN is a soft computing technique that is developed based on the structure of the human brain. Neurons are interconnected within the nervous system and the human brain to solve problems in real-life. An ANN comprises several (or many) neurons, and each neuron has an input/output characteristic and implements a local function or computation (Hajian and Styles 2018). In ANNs, neurons are connected through the network function, and they process data by mapping them from the input to output data streams (Azoff 1994). The performance of the ANN model can be controlled by monitoring the values between connections (i.e., weight and bias) (Schalkoff 2011). For an ANN, all input parameters are collected at the hidden layers, i.e., at each hidden neurons/nodes, via weights. Bias is the sum of hidden neurons/nodes. A specific function can be applied to transform biases (Van Gerven and Bohte 2018), which are then transferred to the next hidden layer(s). Finally, the outcomes are computed in the output layer based on the transformations and targets. Figure 4 illustrates the general structure of an ANN model to predict GCV herein.

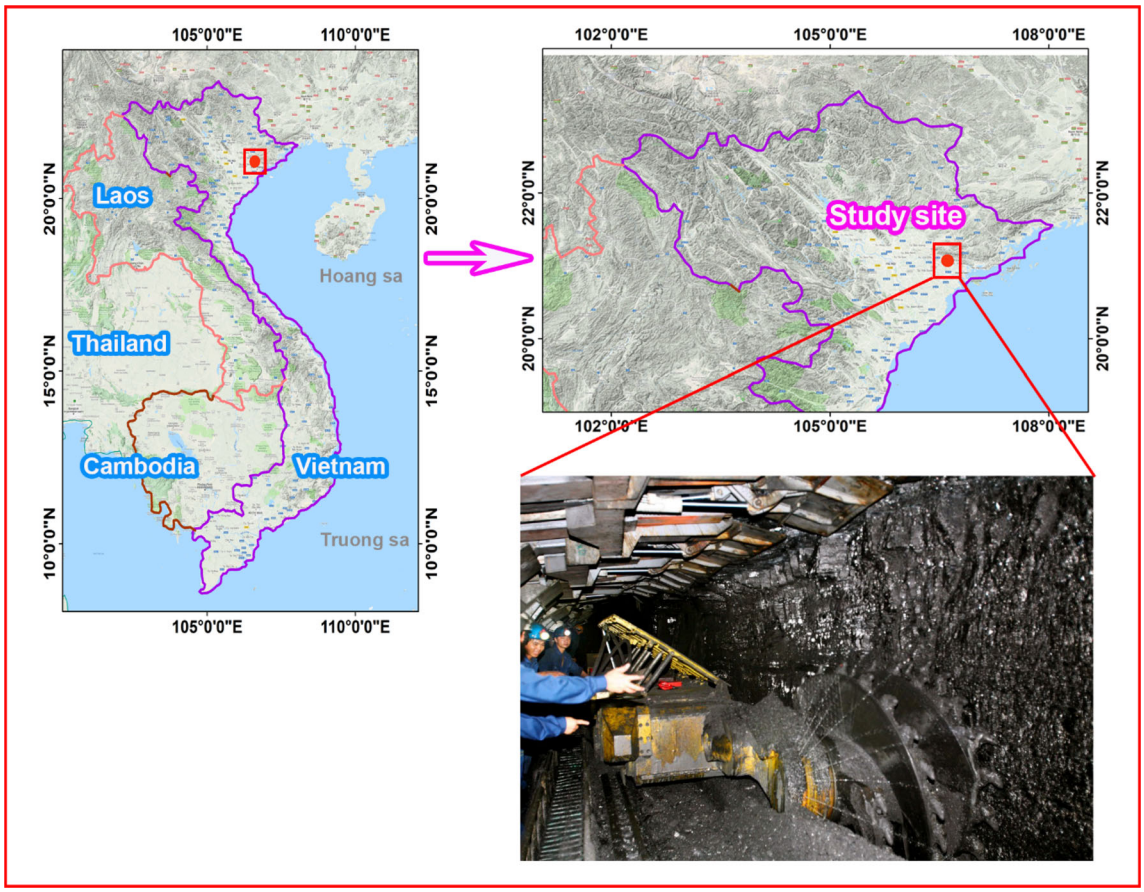

Figure 1. Location of the Mong Duong underground coal mine.

Particle Swarm Optimization

Eberhart and Kennedy (1995) introduced the PSO algorithm as a stochastic optimization technique, which simulates the social behaviors of groups of animals, such as herds, fish, and swarms of birds or insects. Animal groups use a collaborative way for finding food sources, in which individuals are continuously changing the search method used to find out the best food sources based on their own experience and that of other members in the swarm (Wang et al. 2018). The PSO algorithm was designed based on an evolutionary algorithm (EA) and artificial life (AL). Like EA, PSO also uses a feature of the swarm, which is concurrently searching a wide-reaching area in the feature space of the objective function being optimized. PSO applies the characteristics of AL for finding the optimal solution. According to Millonas (1993), the swarm AL model that employs a collaborative behavior was based on five basic principles:

1. Proximity: the swarm implements simple time and space computations.
2. Quality: the swarm can sense the difference in environmental quality and give feedback based on it.
3. Different response: the swarm does not limit the methods of acquiring resources to a narrow bound.
4. Stability: the behavior of the swarm does not change according to the environmental fluctuations.
5. Adaptability: the behavior of the swarm change with a good chance. Note that this opposes the fourth principle.

PSO can update their locations and velocity of particles to meet the quality and proximity requirements in the PSO algorithm, depending on the change in the environment. This action enables the swarm to find the optimal solution in a global search space continuously. In PSO, particles can keep their

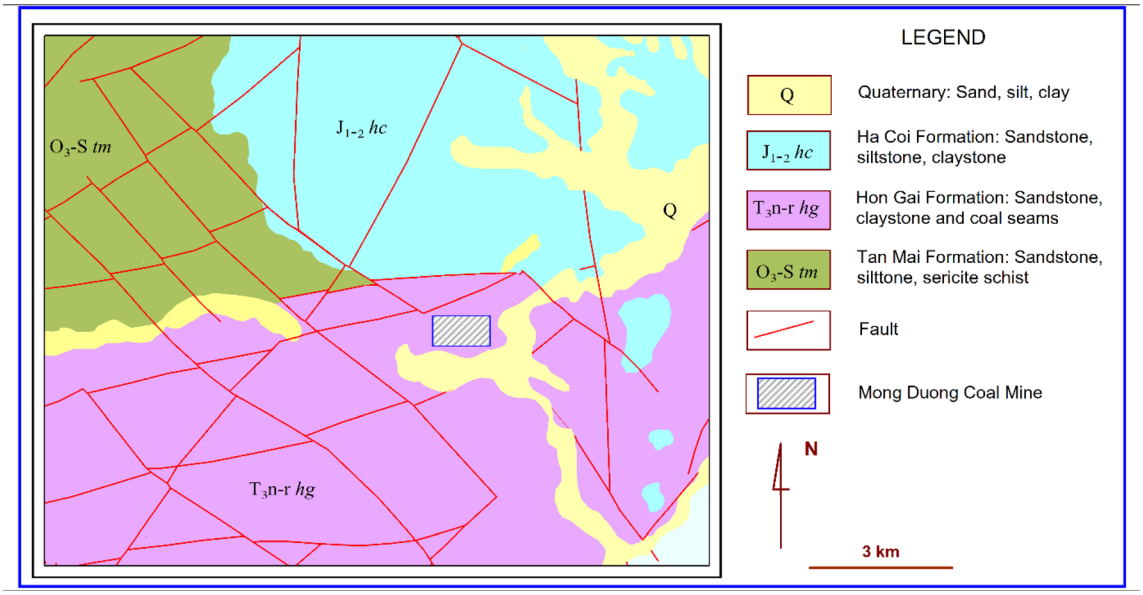

Figure 2. Geological structures and stratigraphic units of the study site.

Table 1. Datasets used in the present study

Obs.	*M* (%)	*A* (%)	VM (%)	GCV (Kcal/kg)
1	0.50	8.60	3.90	6831
2	0.60	19.80	4.30	6393
3	0.20	24.40	5.20	6286
…	…	…	…	…
1017	1.88	10.80	11.30	7424
1018	2.22	10.33	5.45	7818
1019	3.01	13.54	9.19	7434
…	…	…	…	…
2154	1.15	22.01	9.04	6523
2155	1.84	25.91	9.38	5738
…	…	…	…	…
2582	1.15	11.48	7.99	7266
2583	1.67	21.08	7.39	6610

velocities while changing their motion in the search space to adjust to the change in the environment. Therefore, the PSO system can satisfy all five principles of AL systems. Figure 5 shows the pseudo-code, which is applied when searching for an optimal solution using the PSO algorithm.

PSO-ANN Model for GCV Estimation

The PSO-ANN model can be developed in two steps:

- Step 1: Developing an initial ANN model with parameters that can be used to control the accuracy of the ANN model (i.e., weights and biases).
- Step 2: Optimizing the parameters of the initial ANN model. In this step, the weights and biases of the developed ANN model were optimized by the PSO algorithm aiming to get better performance of the ANN model, called PSO-ANN model.

Herein, M, A, and VM were considered as the model inputs for estimating GCV as described above. In the first stage, the training dataset with the input/output parameters, seven ANN models will be developed. Subsequently, the best ANN model is selected for PSO-ANN optimization. Root-mean-squared error (RMSE) function (Eq. 2) is used as an objective function for evaluating the performance of the optimization process of the proposed PSO-ANN model. The process that reached the lowest RMSE is the best performance of the proposed PSO-ANN model. Finally, the testing dataset was used to validate the performance of the optimized PSO-ANN model. Figure 6 shows the flowchart of the proposed PSO-ANN model for predicting GCV.

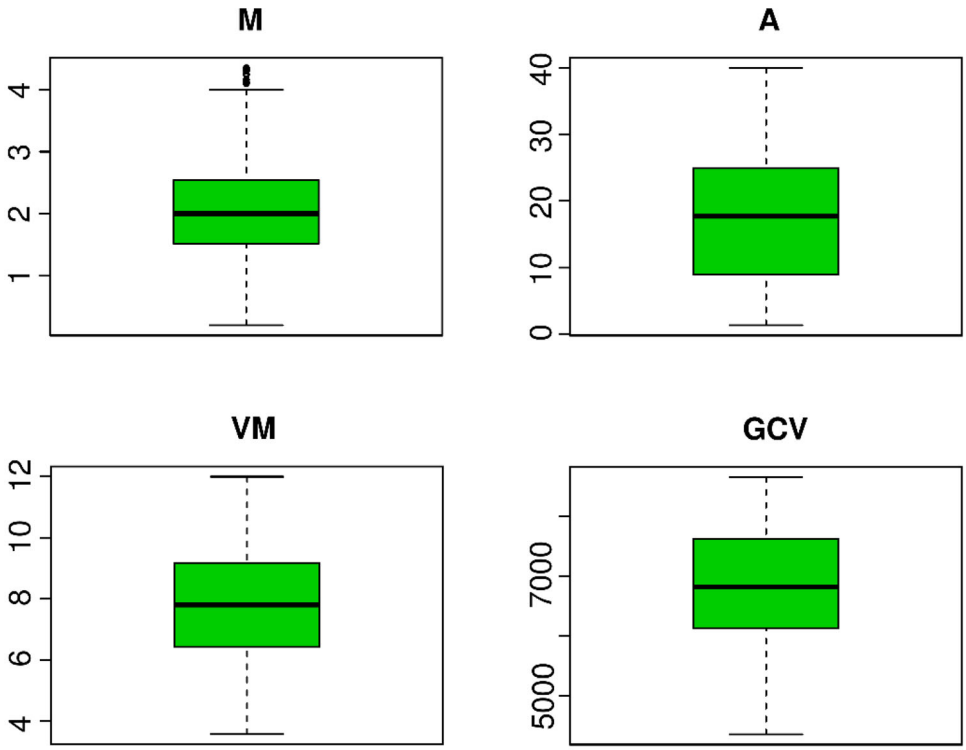

Figure 3. Data used for the GCV prediction.

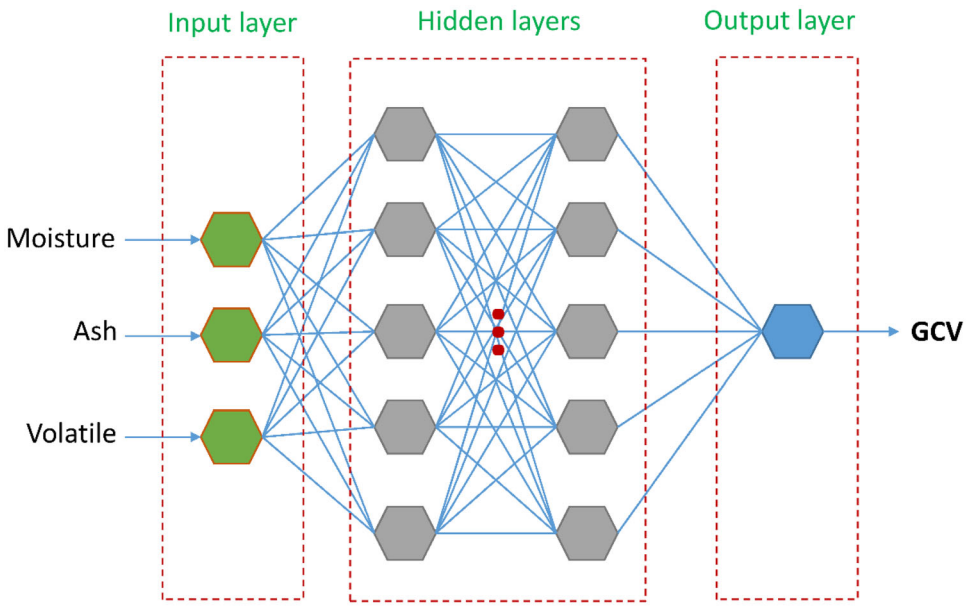

Figure 4. ANN structure for GCV prediction in the present study.

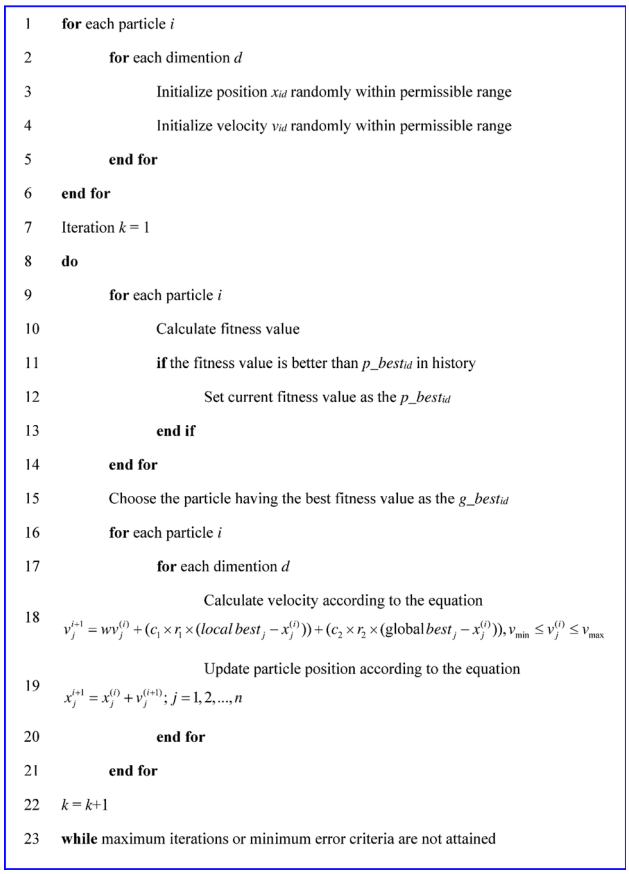

Figure 5. Step-by-step procedure of the PSO algorithm (Kulkarni and Venayagamoorthy 2007).

Model Assessment

The models were assessed using four statistic factors, including RMSE, mean absolute percentage error (MAPE), determination coefficient (R^2), and variance accounted for (VAF). They are calculated as follows (Eqs. 2–5):

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{k=1}^{n}(y_k - \hat{y}_k)^2} \tag{2}$$

$$\text{MAPE} = \frac{100\%}{n}\sum_{k=1}^{n}\left|\frac{y_k - \hat{y}_k}{y_k}\right| \tag{3}$$

$$R^2 = 1 - \frac{\sum_k (y_k - \hat{y}_k)^2}{\sum_k (y_k - \overline{y})^2} \tag{4}$$

$$\text{VAF} = \left(1 - \frac{\text{var}\,(y_k - \hat{y}_k)}{\text{var}\,(y_k)}\right) \times 100 \tag{5}$$

where n represents the total number of data; y_k, $\hat{y}_k$, and $\overline{y}$ are measured, predicted, and mean of y_k values, respectively. To highlight and classify the developed models based on the performance indices, the color intensity (as illustrated below) and ranking of the individual models were used.

DEVELOPMENT OF ANN MODELS FOR GCV PREDICTION

First, the dataset used in the ANN model development was randomly divided into two groups. Previous studies showed that an 80/20 dividing ratio

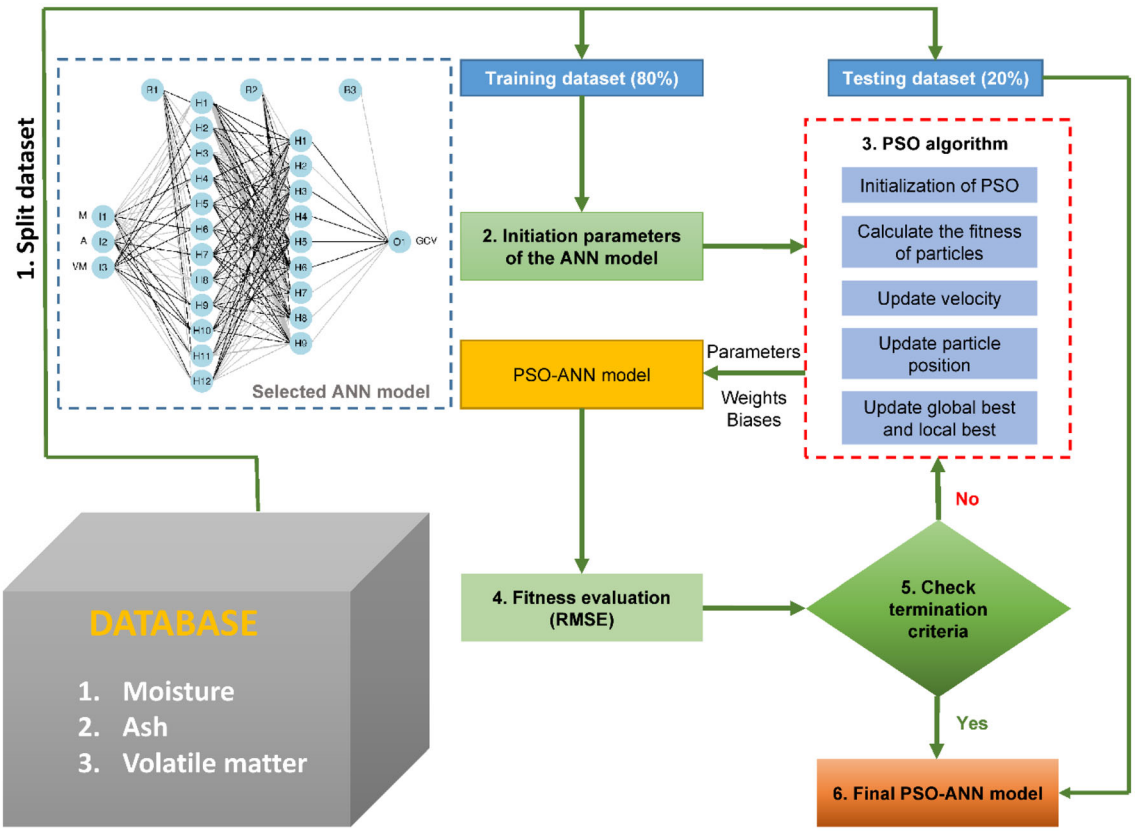

Figure 6. Proposed novel AI system for estimation of GCV (PSO-ANN).

is suitable for training and testing the AI models (Nguyen et al. 2018; Bui et al. 2019c, d; Nguyen et al. 2019c). Therefore, the dataset used in this study was randomly divided between the two groups according to this ratio (Fig. 6). It is worth noting that the MinMax scale [− 1, 1] and tenfold cross-validation techniques were used to avoid the over-fitting of the ANN and PSO-ANN models.

Next, the structure of ANN models was designed, which is not a simple process. Figure 4 shows that the hardest step in the process is to create the hidden layer(s) and hidden neuron(s), because several hidden layers/neurons may lead to over-fitting/under-fitting (Nguyen et al. 2018), which is a time-consuming process(Nguyen et al. 2019d). Therefore, we followed a trial and error procedure, and the ANN models were based on one, two, and three hidden layers, assuming that the hidden neurons exist in the range between 2 and 13. The training dataset (2068 observations) was used for modeling GCV by ANNs. The seven ANN models that were designed in this study are as follows: ANN 3-7-1, ANN 3-8-1, ANN 3-9-1, ANN 3-7-4-1, ANN 3-12-9-1, ANN 3-8-5-2-1, and ANN 3-13-9-6-1 (Fig. 7).

The performance of the seven ANN models was assessed through RMSE, R^2, VAF, and MAPE. They were ranked using the color intensity technique to evaluate their quality on the training dataset. Table 2 calculates the performance indices of the designed ANN models.

The results of Table 2 indicate that all the performances of ANN models were excellent in estimating GCV. ANN 3-12-9-1 showed the best performance with the maximum red color intensity. In contrast, ANN 3-7-1 showed the worst performance with minimum red color intensity. In addition, ANN models containing two or three hidden layers performed better compared to those containing one hidden layer. Figure 8 indicates how different between the predicted and measured GCV values by individual models on the process of training.

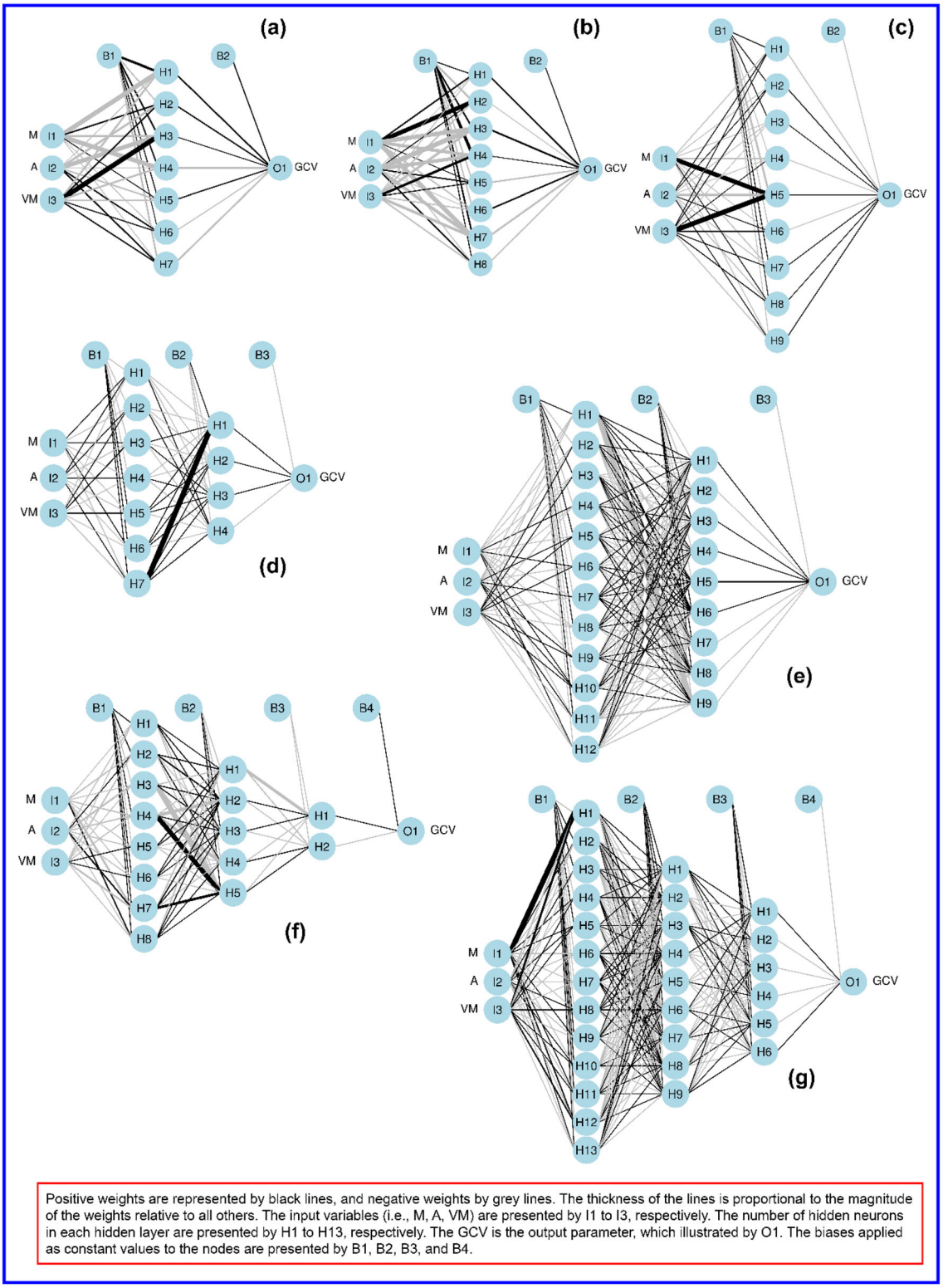

Figure 7. Structure design of the ANN models for GCV prediction: (a) ANN 3-7-1; (b) ANN 3-8-1; (c) ANN 3-9-1; (d) ANN 3-7-4-1; (e) ANN 3-12-9-1; (f) ANN 3-8-5-2-1; (g) ANN 3-13-9-6-1.

PSO of Selected ANN model (PSO-ANN)

The optimization was performed on the best ANN model (i.e., ANN 3-12-9-1) using the PSO algorithm. Only weights and biases of the selected ANN model are optimized using PSO to improve its performance. The first step in this process was setting the parameters of PSO algorithm, in which the initialization parameters were: the number of swarm particles (p), maximum velocity of the particle (V_{max}), individual cognitive (ϕ_1), group cognitive (ϕ_2), and inertia weight (w). According to Agrawal and Kaur (2018), p has to reflect the diversity of the swarm; thus, it was set to 50, 100, 15, 200, 250 in this study. Kennedy (2002) recommended setting ϕ_1 and ϕ_2 at the same values so that they satisfy the following condition: $0<\phi_1+\phi_2<4$. Therefore, here they were both set at 1.5. The balance between the local and global search was ensured by setting w to 0.9. To ensure convergence and prevent an explosion, V_{max} was set to 2. The maximum iterations (m_i) were set to 500 to ensure the convergence of the model, and RMSE using Eq. 1, which was used as a fitness function to examine the performance of the proposed PSO-ANN model. The optimization process of the ANN 3-12-9-1 model by the PSO algorithm is shown in Figure 9. Finally, the optimal PSO-ANN model was obtained at p = 150 and m_i = 135. The other parameters of the PSO algorithm were as mentioned above. The new improved ANN model was then developed and called the PSO-ANN model (Fig. 10). It is worth mentioning that the structures of the ANN models in Figures 10 and 7e are similar, but their weights and biases are different. In other words, the structure of the improved ANN model in Figure 10 was optimized than those of the ANN model in Figure 7e.

A comparison was then conducted between the performance before and after the optimization using RMSE, R^2, VAF, and MAPE (Table 3). The results showed that the proposed PSO-ANN model performed better than the best selected ANN model (ANN 3-12-9-1) without optimization on the training dataset. Figure 11 demonstrates the performances of the optimization process using PSO and the selected ANN model (without optimization) on the training dataset.

EXPERIMENT RESULTS AND DISCUSSIONS

The performances of the proposed PSO-ANN and the seven ANN models are examined and evaluated via the testing dataset (515 samples). Table 4 shows the results of the evaluation techniques, which were similar to those used in the evaluation of the models on the training dataset.

Table 4 shows the results of the proposed PSO-ANN model that yielded the best performance because these results are superior to those predicted with the other ANN models. It can be seen that there are three outstanding models for predicting GCV in Table 4 with high intensity of the red color,

Table 2. Training performance of the models

Model	Performance metrics				Rank for RMSE	Rank for R^2	Rank for VAF	Rank for MAPE	Total rank
	RMSE	R^2	VAF	MAPE					
ANN 3-7-1	207.587	0.954	95.355	0.018	1	1	1	1	4
ANN 3-8-1	202.462	0.956	95.582	0.017	2	2	2	3	9
ANN 3-9-1	200.001	0.957	95.689	0.017	3	3	3	4	13
ANN 3-7-4-1	196.439	0.958	95.841	0.018	4	4	4	2	14
ANN 3-12-9-1	187.432	0.962	96.214	0.017	7	7	7	6	27
ANN 3-8-5-2-1	191.184	0.961	96.060	0.017	5	5	5	7	22
ANN 3-13-9-6-1	189.945	0.961	96.111	0.017	6	5	6	5	22

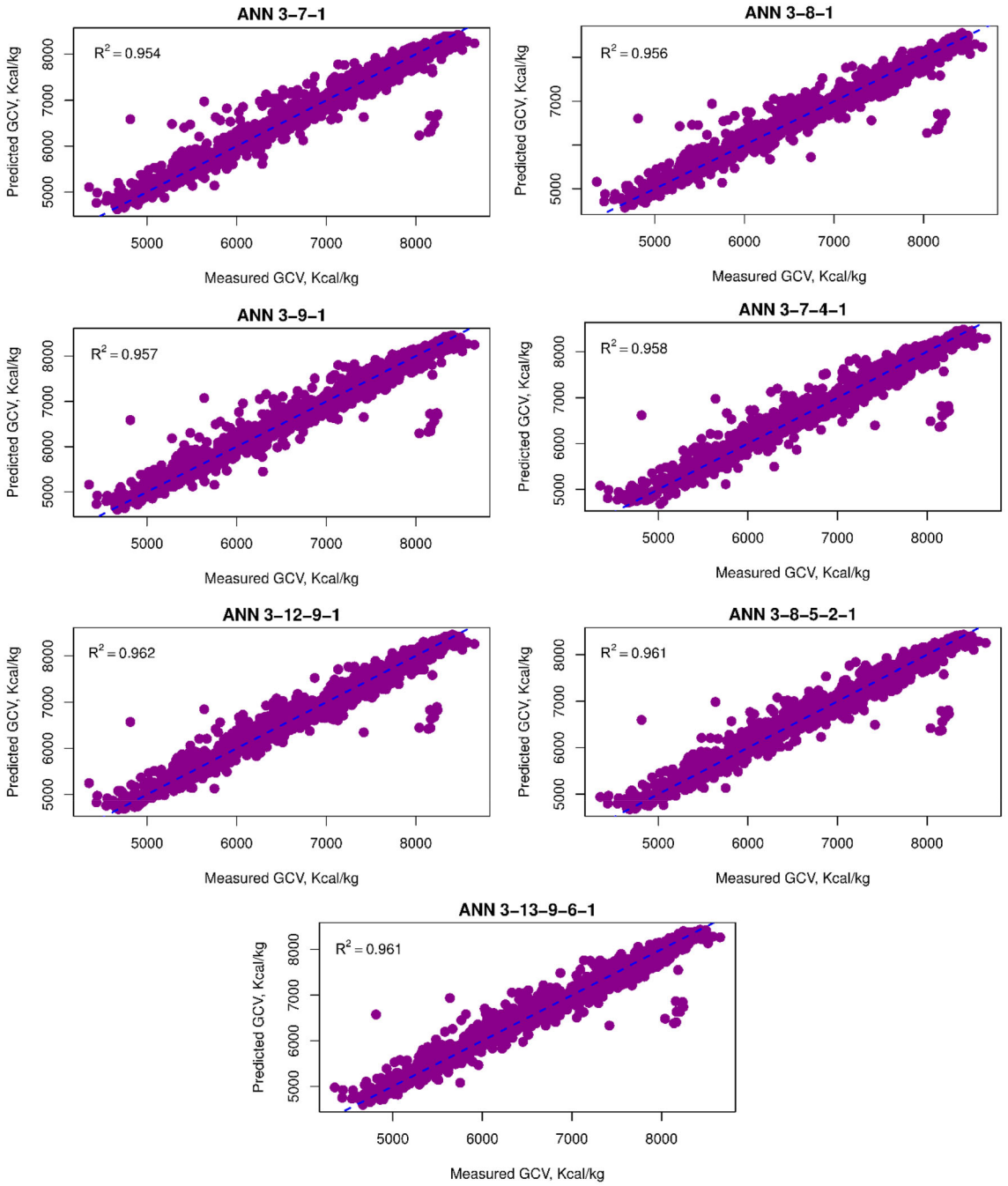

Figure 8. Plots of measured vs. predicted GCVs in the training process.

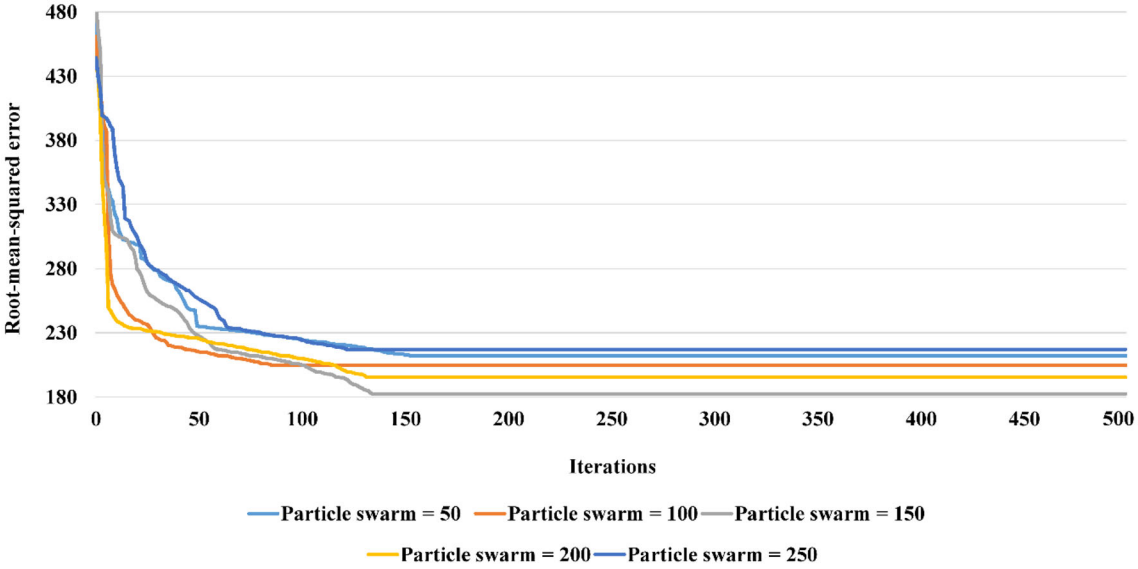

Figure 9. Optimization of the selected ANN model by the PSO algorithm.

including the ANN 3-12-9-1, ANN 3-13-9-6-1, and the PSO-ANN models. Of those, the PSO-ANN model provided the most dominant color intensity, and the total ranking indicated the same results (i.e., a total ranking of 27). Comparing the performance between the best ANN model, which is selected in Table 3 and the PSO-ANN model on the testing dataset, we can see that the performance of the PSO-ANN model is also much better than those of the ANN 3-12-9-1 model. These findings confirmed the performance, as well as the reliability of the proposed PSO-ANN in practical engineering.

Furthermore, a comprehensive comparison and evaluation of ANN models were interpreted based on the results listed in Table 4, which revealed that not all ANN models with several hidden layers are efficient. For example, the performance of the ANN 3-13-9-6-1 model even was less than that of the ANN 3-7-1, ANN 3-8-1, ANN 3-7-4-1, and ANN 3-12-9-1 models, with the total ranking of only 7. These results show that the performance of the ANN 3-13-9-6-1 model may be affected by too many hidden layers with fewer hidden neurons. Nguyen et al. (2018) also recommended that the ANN model may have been under-fitting or over-fitting if using too many hidden layers or fewer hidden neurons. However, comparing the results on both training and testing datasets can see that the ANN 3-13-9-6-1 model is not over-fitting or under-fitting in this case study. Its performance is lower only when compared to those of the other models on the testing dataset. This can be attributed to the transmission of information between neurons and hidden layers via weights and biases. Figure 12 shows an assessment of the models on the testing dataset via R^2. This assessment revealed that the optimization using the PSO algorithm has helped to improve the accuracy of the ANN model in predicting GCV, i.e., PSO-ANN model. Therefore, it provides a powerful search and optimization solution for weights and biases of the ANN model.

As stated in the data collection section, GCV values were determined by the Bomb calorimeter (Model Parr 6200), and it took 6 min per sample. Herein, this study used 2583 samples for training and testing the performance of the GCV predictive models. Of those, 515 samples were used for the testing process. Whereas, the proposed PSO-ANN model in this study took only 2-3 s to estimate the GCV of 515 samples based on the developed model. That is the most superior advantage of AI models compared with the experimental methods as well.

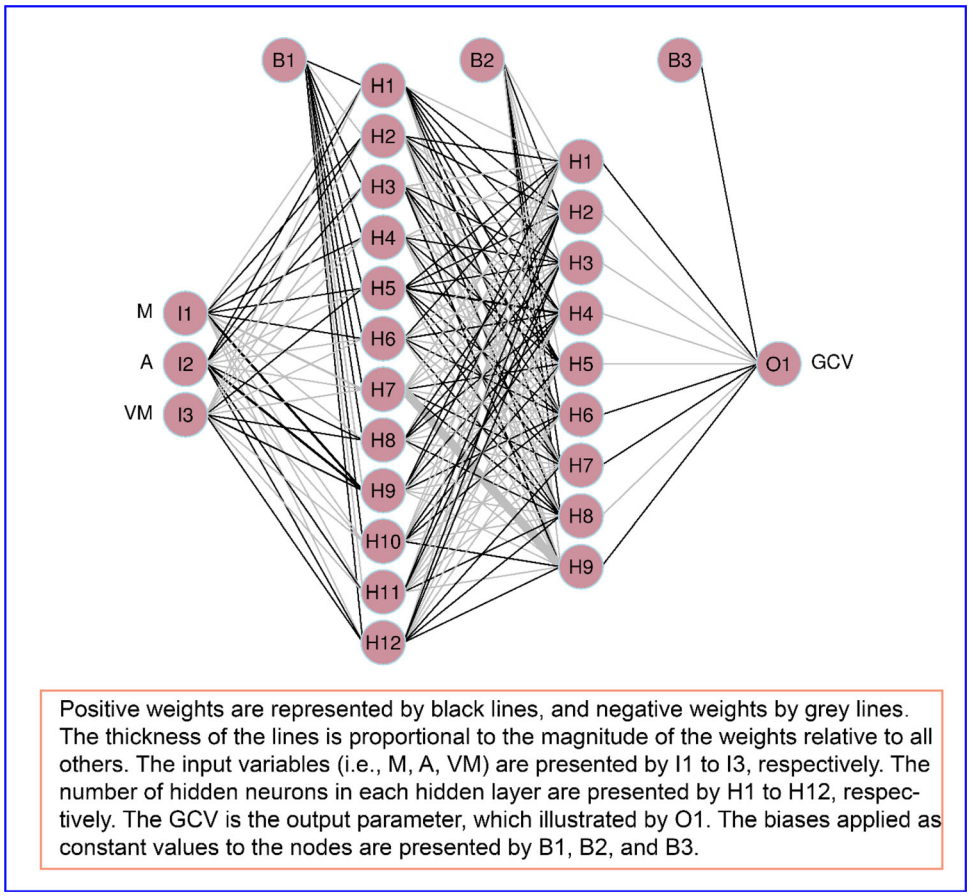

Figure 10. Structure of the proposed PSO-based ANN model (after being optimized).

Table 3. Comparison (based on the training dataset) between the selected ANN model before and after optimization

Model	Performance metrics			
	RMSE	R^2	VAF	MAPE
Selected ANN	187.432	0.962	96.214	0.017
PSO-ANN	182.476	0.964	96.411	0.016

In machine learning, the only training time of AI models is concerned and measured to evaluate the computational cost of the models. However, the training time is recommended that is highly dependent on the structure of the hardware of the computer used (Madiajagan and Raj 2019; Bacchus et al. 2020). Therefore, the significance is low in evaluating the performance of the models if using the training time. In this study, a workstation computer with the processor Xeon-X5675, 24 GB RAM, and 64-bit operating system was used to develop the ANN and PSO-ANN models. Of those, the maximum training time is 2534 s for the PSO-ANN model. Whereas, the remaining ANN models took around 29–61 s. However, 2534 s for developing a predictive model with big data is not high, and as addressed above, once the predictive model was well-developed, it can predict GCV values rapidly (only 2–3 s). For example, this study used 2068 samples to develop the PSO-ANN model; then, it took 2–3 s to estimate the GCV value of 515 samples in the testing dataset. Meanwhile, it will take about 515 * 6 min = 3090 min (~ 51.5 h) to determine GCV values by the bomb calorimeter. Therefore, the proposed PSO-ANN model was introduced as a rapid determi-

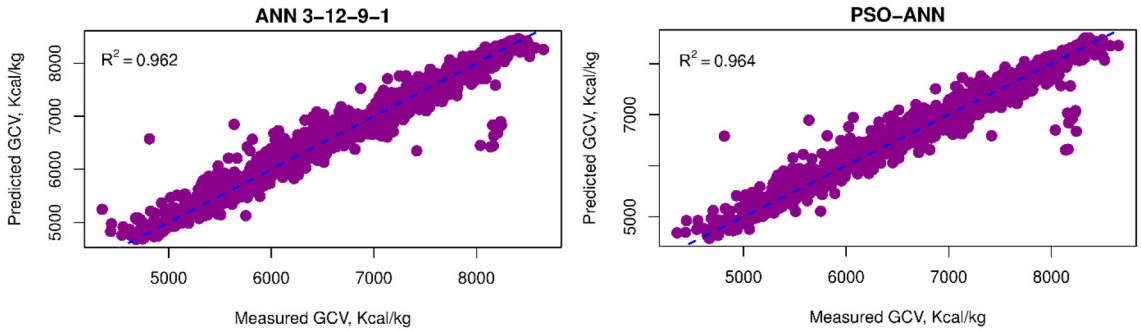

Figure 11. Measured vs. predicted GCV values by the selected ANN model before and after optimization by PSO algorithm on the training dataset.

Table 4. The testing performance of the models

Model	Performance metrics				Rank for RMSE	Rank for R^2	Rank for VAF	Rank for MAPE	Total rank
	RMSE	R^2	VAF	MAPE					
ANN 3-7-1	212.775	0.950	95.014	0.018	1	1	1	7	10
ANN 3-8-1	208.444	0.952	95.215	0.018	3	2	3	5	13
ANN 3-9-1	208.102	0.952	95.230	0.018	4	2	4	7	17
ANN 3-7-4-1	203.993	0.954	95.416	0.019	5	5	5	1	16
ANN 3-12-9-1	201.155	0.955	95.543	0.018	7	6	7	4	24
ANN 3-8-5-2-1	209.212	0.952	95.178	0.019	2	2	2	1	7
ANN 3-13-9-6-1	202.603	0.955	95.478	0.019	6	6	6	3	21
PSO-ANN	199.891	0.956	95.598	0.018	7	7	7	6	27

nation method for estimating the GCV of coal in this study.

CONCLUSIONS

GCV is an important indicator to assess the quality of coal used as fuel. GCV can be accurately predicted by AI techniques based on several factors, such as moisture, ash, and VM. Predicting accurate GCV helps mining engineers classify coal based on the application and improve the efficiency of selective extraction. Additionally, GCV is also an essential basis for calculating input materials for thermal and metallurgical plants. The following conclusions are drawn from the results of this study:

- AI techniques can be used for predicting GCV that has high accuracy and reliability based on the contents of moisture, ash, VM, and FC, particularly through ANN.
- The PSO algorithm is a powerful optimization tool that should be used to optimize ANN to increase the accuracy of the GCV predictions.
- The proposed PSO-ANN model, which is a robust soft computing model, predicts the GCV of coal. Thus, it should be used as an alternative technique in practical engineering for determining GCV.

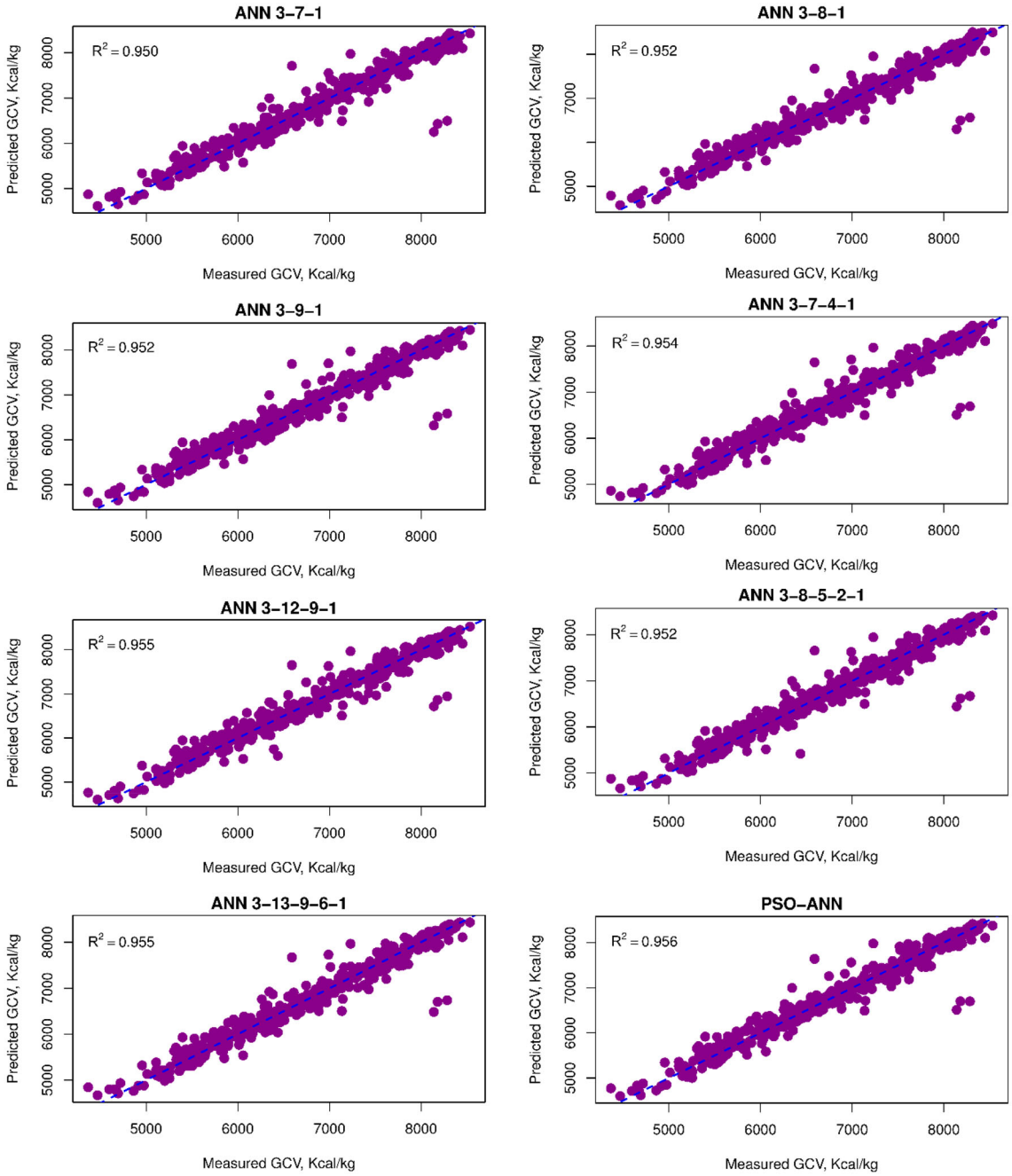

Figure 12. Plots of measured vs. predicted GCVs in the testing process.

ACKNOWLEDGMENTS

This paper was supported by the Center for Mining, Electro-Mechanical research of Hanoi University of Mining and Geology (HUMG), Hanoi, Vietnam, and the research team of Innovations for Sustainable and Responsible Mining (ISRM) of HUMG.

REFERENCES

Agrawal A. P., & Kaur A., (2018) A comprehensive comparison of ant colony and hybrid particle swarm optimization algorithms through test case selection. In: S. Satapathy, V. Bhateja, K. Raju, B. Janakiramaiah (Eds.) *Data engineering and intelligent computing*. Advances in intelligent systems and computing (Vol. 542). Singapore: Springer. https://doi.org/10.1007/978-981-10-3223-3_38.

Andres, J., & Bona, M. (2005). Analysis of coal by diffuse reflectance near-infrared spectroscopy. *Analytica Chimica Acta, 535*(1–2), 123–132.

Azoff, E. M. (1994). *Neural network time series forecasting of financial markets*. New York: Wiley.

Bacchus, P., Stewart, R., & Komendantskaya, E. (2020). Accuracy, training time and hardware efficiency trade-offs for quantized neural networks on FPGAs. In *International symposium on applied reconfigurable computing, 2020* (pp. 121–135). Berlin: Springer.

Baghban, A., & Ebadi, T. (2019). GA-ANFIS modeling of higher heating value of wastes: Application to fuel upgrading. *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, 41*(1), 7–13.

Balaeva, Y. S., Miroshnichenko, D., & Kaftan, Y. S. (2018). Method for calculating the gross calorific value of coal on a moist ash-free basis. *Solid Fuel Chemistry, 52*(5), 279–288.

Begum, N., Chakravarty, D., & Das, B. S. (2019). Estimation of gross calorific value of bituminous coal using various coal properties and reflectance spectra. *International Journal of Coal Preparation and Utilization*. https://doi.org/10.1080/19392699.2019.1621301.

Bhatt, A., Priyadarshini, S., Mohanakrishnan, A. A., Abri, A., Sattler, M., & Techapaphawit, S. (2019). Physical, chemical, and geotechnical properties of coal fly ash: A global review. *Case Studies in Construction Materials, 11,* e00263.

Bui, X.-N., Jaroonpattanapong, P., Nguyen, H., Tran, Q.-H., & Long, N. Q. (2019a). A novel hybrid model for predicting blast-induced ground vibration based on k-nearest neighbors and particle swarm optimization. *Scientific Reports, 9*(1), 1–14.

Bui, D. T., Khosravi, K., Karimi, M., Busico, G., Khozani, Z. S., Nguyen, H., et al. (2020a). Enhancing nitrate and strontium concentration prediction in groundwater by using new data mining algorithm. *Science of the Total Environment, 715*, 136836. https://doi.org/10.1016/j.scitotenv.2020.136836.

Bui, D. T., Khosravi, K., Karimi, M., Busico, G., Khozani, Z. S., Nguyen, H., et al. (2020). Enhancing nitrate and strontium concentration prediction in groundwater by using new data mining algorithm. Science of the Total Environment, 715, 136836. doi: 10.1016/j.scitotenv.2020.136836.

Bui, X.-N., Muazu, M. A., & Nguyen, H. (2020b). Optimizing Levenberg–Marquardt backpropagation technique in predicting factor of safety of slopes after two-dimensional OptumG2 analysis. *Engineering with Computers, 36*(3), 941–952.

Bui, H.-B., Nguyen, H., Choi, Y., Bui, X.-N., Nguyen-Thoi, T., & Zandi, Y. (2019c). A Novel artificial intelligence technique to estimate the gross calorific value of coal based on meta-heuristic and support vector regression algorithms. *Applied Sciences, 9*(22), 4868.

Bui, X.-N., Nguyen, H., Le, H.-A., Bui, H.-B., & Do, N.-H. (2019d). Prediction of blast-induced air over-pressure in open-pit mine: Assessment of different artificial intelligence techniques. *Natural Resources Research, 29*(2), 571–591.

Bustin, R. M., Mastalerz, M., & Wilks, K. R. (1993). Direct determination of carbon, oxygen and nitrogen content in coal using the electron microprobe. *Fuel, 72*(2), 181–185.

Carraher, C. E., Jr. (2017). *Carraher's polymer chemistry*. Boca Raton: CRC Press.

Dong, M., Lu, J., Yao, S., Li, J., Li, J., Zhong, Z., et al. (2011). Application of LIBS for direct determination of volatile matter content in coal. *Journal of Analytical Atomic Spectrometry, 26*(11), 2183–2188.

Dung, N. T. K., Son, N. H., Chinh, V. T., & Duoc, T. V. (2020). Study on the effects of some parameters on the flotation performance of Vang Danh coal fines −0.3 mm in the reflux flotation cell (in Vietnamese). *Journal of Mining and Earth Sciences, 61*(02), 68–75.

Duoc, T. V., Son, N. H., Dung, N. T. K., & Chinh, V. T. (2020). Recovery of clean coal from blast furnace dusts by flotation column (in Vietnamese). *Journal of Mining and Earth Sciences, 61*(01), 124–131.

Eberhart, R., & Kennedy, J. (1995). A new optimizer using particle swarm theory. In *MHS'95. proceedings of the sixth international symposium on micro machine and human science, 1995* (pp. 39–43). IEEE.

Fagerbakke, K. M., Heldal, M., & Norland, S. (1996). Content of carbon, nitrogen, oxygen, sulfur and phosphorus in native aquatic and cultured bacteria. *Aquatic Microbial Ecology, 10*(1), 15–27.

Feng, Q., Zhang, J., Zhang, X., & Wen, S. (2015). Proximate analysis based prediction of gross calorific value of coals: A comparison of support vector machine, alternating conditional expectation and artificial neural network. *Fuel Processing Technology, 129,* 120–129.

Given, P. H., Weldon, D., & Zoeller, J. H. (1986). Calculation of calorific values of coals from ultimate analyses: theoretical basis and geochemical implications. *Fuel, 65*(6), 849–854.

Gómez, Y. R., Hernández, R. C., Guerrero, J. E., & Mejía-Ospino, E. (2018). FTIR-PAS coupled to partial least squares for prediction of ash content, volatile matter, fixed carbon and calorific value of coal. *Fuel, 226,* 536–544.

Guo, H., Nguyen, H., Bui, X.-N., & Armaghani, D. J. (2019a). A new technique to predict fly-rock in bench blasting based on an ensemble of support vector regression and GLMNET. *Engineering with Computers*. https://doi.org/10.1007/s00366-019-00833-x.

Guo, H., Nguyen, H., Vu, D.-A., & Bui, X.-N. (2019b). Forecasting mining capital cost for open-pit mining projects based on artificial neural network approach. *Resources Policy*. https://doi.org/10.1016/j.resourpol.2019.101474.

Hadavandi, E., Hower, J. C., & Chelgani, S. C. (2017). Modeling of gross calorific value based on coal properties by support vector regression method. *Modeling Earth Systems and Environment, 3*(1), 37.

Hajian, A., & Styles, P. (2018). *Application of soft computing and intelligent methods in geophysics*. Berlin: Springer.

Jorjani, E., Poorali, H. A., Sam, A., Chelgani, S. C., Mesroghli, S., & Shayestehfar, M. (2009). Prediction of coal response to froth flotation based on coal analysis using regression and artificial neural network. *Minerals Engineering, 22*(11), 970–976.

Küçükbayrak, S., Dürüs, B., Meríçboyu, A. E., & Kadioğlu, E. (1991). Estimation of calorific values of Turkish lignites. *Fuel, 70*(8), 979–981.

Kulkarni, R. V., & Venayagamoorthy, G. K. (2007). An estimation of distribution improved particle swarm optimization algorithm. In *2007 3rd international conference on intelligent sensors, sensor networks and information* (pp. 539–544). IEEE.

Le, B. T., Xiao, D., Mao, Y., & He, D. (2018). Coal analysis based on visible-infrared spectroscopy and a deep neural network. *Infrared Physics & Technology, 93,* 34–40.

Liu, P., & Lv, S. (2020). Measurement and calculation of calorific value of raw coal based on artificial neural network analysis method. *Thermal Science*(00), 87-87.

Lu, Z., Chen, X., Yao, S., Qin, H., Zhang, L., Yao, X., et al. (2019). Feasibility study of gross calorific value, carbon content, volatile matter content and ash content of solid biomass fuel using laser-induced breakdown spectroscopy. *Fuel, 258,* 116150.

Lu, Z., Mo, J., Yao, S., Zhao, J., & Lu, J. (2017). Rapid determination of the gross calorific value of coal using laser-induced breakdown spectroscopy coupled with artificial neural networks and genetic algorithm. *Energy & Fuels, 31*(4), 3849–3855.

Madiajagan, M., & Raj, S. S. (2019). Chapter 1 - Parallel computing, graphics processing unit (GPU) and new hardware for deep learning in computational intelligence research. In A. K. Sangaiah (Ed.), *Deep learning and parallel computing environment for bioengineering systems* (pp. 1–15). Academic Press.

Majumder, A. K., Jain, R., Banerjee, P., & Barnwal, J. (2008). Development of a new proximate analysis based correlation to predict calorific value of coal. *Fuel, 87*(13–14), 3077–3081.

Mason, D. M., & Gandhi, K. N. (1983). Formulas for calculating the calorific value of coal and coal chars: Development, tests, and uses. *Fuel Processing Technology, 7*(1), 11–22.

Matin, S., & Chelgani, S. C. (2016). Estimation of coal gross calorific value based on various analyses by random forest method. *Fuel, 177,* 274–278.

Mesroghli, S., Jorjani, E., & Chelgani, S. C. (2009). Estimation of gross calorific value based on coal analysis using regression and artificial neural networks. *International Journal of Coal Geology, 79*(1–2), 49–54.

Millonas, M. M. (1993). Swarms, phase transitions, and collective intelligence. *arXiv preprint adap-org/9306002*.

Musa, N., Usaku, R., Akinterinwa, A., & Maina, H. (2018). Studies on elemental composition and physico-chemical properties of coal deposits in Lamza and Guyuk Local Government, Adamawa State, Nigeria. *Bayero Journal of Pure and Applied Sciences, 11*(2), 267–273.

Nguyen, H. (2019). Support vector regression approach with different kernel functions for predicting blast-induced ground vibration: a case study in an open-pit coal mine of Vietnam. *SN Applied Sciences, 1*(4), 283.

Nguyen, H., & Bui, X.-N. (2020). Soft computing models for predicting blast-induced air over-pressure: A novel artificial intelligence approach. *Applied Soft Computing, 92,* 106292.

Nguyen, H., Bui, X.-N., Bui, H.-B., & Cuong, D. T. (2019a). Developing an XGBoost model to predict blast-induced peak particle velocity in an open-pit mine: A case study. *Acta Geophysica, 67*(2), 477–490.

Nguyen, H., Bui, X.-N., Bui, H.-B., & Mai, N.-L. (2018). A comparative study of artificial neural networks in predicting blast-induced air-blast overpressure at Deo Nai open-pit coal mine, Vietnam. *Neural Computing and Applications*. https://doi.org/10.1007/s00521-018-3717-5.

Nguyen, H., Bui, X.-N., Bui, H.-B., & Mai, N.-L. (2020). A comparative study of artificial neural networks in predicting blast-induced air-blast overpressure at Deo Nai open-pit coal mine, Vietnam. *Neural Computing and Applications, 32*(8), 3939–3955.

Nguyen, H., Bui, X.-N., & Moayedi, H. (2019b). A comparison of advanced computational models and experimental techniques in predicting blast-induced ground vibration in open-pit coal mine. *Acta Geophysica, 67*(4), 1025–1037.

Nguyen, H., Bui, X.-N., Tran, Q.-H., & Mai, N.-L. (2019c). A new soft computing model for estimating and controlling blast-produced ground vibration based on hierarchical K-means clustering and cubist algorithms. *Applied Soft Computing, 77,* 376–386.

Nguyen, H., Drebenstedt, C., Bui, X.-N., & Bui, D. T. (2019d). Prediction of blast-induced ground vibration in an open-pit mine by a novel hybrid model based on clustering and artificial neural network. *Natural Resources Research, 29*(2), 691–709.

Nguyen, H., Mehrabi, M., Kalantar, B., Moayedi, H., & Abdullahi, M. A. M. (2019e). Potential of hybrid evolutionary approaches for assessment of geo-hazard landslide susceptibility mapping. *Geomatics, Natural Hazards and Risk, 10*(1), 1667–1693.

Nhu, H. V., Duong, B. V., Vo, T. A., & Pham, K. T. (2020). Using numerical modeling method for design and constructive controlling of excavation wall in Madison Building, Ho Chi Minh city. *Journal of Mining and Earth Sciences, 61*(03), 19–27.

Onifade, M., Lawal, A. I., Aladejare, A. E., Bada, S., & Idris, M. A. (2019). Prediction of gross calorific value of solid fuels from their proximate analysis using soft computing and regression analysis. *International Journal of Coal Preparation and Utilization*. https://doi.org/10.1080/19392699.2019.1695605.

Parr, I. C. (2020). Description of the 6200 Isoperibol Calorimeter. Retrieved March 15, 2020, from https://www.parrinst.com/products/oxygen-bomb-calorimeters/6200-isoperibol-calorimeter/.

Patel, S. U., Kumar, B. J., Badhe, Y. P., Sharma, B., Saha, S., Biswas, S., et al. (2007). Estimation of gross calorific value of coals using artificial neural networks. *Fuel, 86*(3), 334–344.

Posom, J., & Sirisomboon, P. (2017). Evaluation of the higher heating value, volatile matter, fixed carbon and ash content of ground bamboo using near infrared spectroscopy. *Journal of Near Infrared Spectroscopy, 25*(5), 301–310.

Schalkoff, R. J. (2011). *Intelligent systems: Principles, paradigms, and pragmatics*. Burlington: Jones & Bartlett Publishers.

Scott, A. R. (2002). Hydrogeologic factors affecting gas content distribution in coal beds. *International Journal of Coal Geology, 50*(1–4), 363–387.

Shirazi, A. R., Börtin, O., Eklund, L., & Lindqvist, O. (1995). The impact of mineral matter in coal on its combustion, and a new approach to the determination of the calorific value of coal. *Fuel, 74*(2), 247–251.

Sivrikaya, O. (2014). Cleaning study of a low-rank lignite with DMS, Reichert spiral and flotation. *Fuel, 119,* 252–258.

Stanger, R., Tran, Q. A., Browne, M., Lucas, J., Naebe, M., Height, M., et al. (2018). Evaluating the thermal extrusion behavior of a coking coal for direct carbon fiber production. *Energy & Fuels, 32*(4), 4528–4537.

Tran, V. T. T. (2020). Dynamic symbol for electronic map, network map and the ability to create dynamic symbol on the map with the online answering machine. *Journal of Mining and Earth Sciences, 61*(03), 85–95.

van Gerven, M., & Bohte, S. (2017). Editorial: Artificial neural networks as models of neural information processing. *Frontiers in Computational Neuroscience*, *11*, 114–114. https://doi.org/10.3389/fncom.2017.00114.

Vassilev, S. V., Baxter, D., Andersen, L. K., & Vassileva, C. G. (2010). An overview of the chemical composition of biomass. *Fuel, 89*(5), 913–933.

Vite, C. (2017). *Report on the results of exploration of Mong Duong coal Mine, Cam Pha City, Quang Ninh province*. Hanoi: General Department of Geology and Minerals of Vietnam.

Wang, D., Tan, D., & Liu, L. (2018). Particle swarm optimization algorithm: an overview. *Soft Computing, 22*(2), 387–408.

Wen, X., Jian, S., & Wang, J. (2017). Prediction models of calorific value of coal based on wavelet neural networks. *Fuel, 199,* 512–522.

Wu, S., Lv, Q., Liu, X., Chen, W., & Che, D. (2017). Study on correlations of coal chemical properties based on database of real-time data. *Applied Energy, 204,* 1115–1123.

Yao, S., Qin, H., Wang, Q., Lu, Z., Yao, X., Yu, Z., et al. (2020). Optimizing analysis of coal property using laser-induced breakdown and near-infrared reflectance spectroscopies. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 239*, 118492. https://doi.org/10.1016/j.saa.2020.118492.

Zhang, H., Nguyen, H., Bui, X.-N., Nguyen-Thoi, T., Bui, T.-T., Nguyen, N., et al. (2020a). Developing a novel artificial intelligence model to estimate the capital cost of mining projects using deep neural network-based ant colony optimization algorithm. *Resources Policy, 66,* 101604.

Zhang, W., Zhuo, Z., Lu, P., Tang, H., Tang, J., Lu, J., et al. (2020b). LIBS analysis of ash content, volatile matter, and calorific value in coal by partial least squares regression based on ash classification. *Journal of Analytical Atomic Spectrometry*. https://doi.org/10.1039/D0JA00186D.