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Determination of the lower calorific and ash values of the lignite coal by using artificial neural networks and multiple regression analysis

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Abstract: The calorific value of coal varies depending on type of coal and foreign matter content. The calorific value of coal from pits is determined by analyzing moisture, volatile matter, ash and sulfur content in laboratories. This analysis process imposes a burden on businesses both in terms of time and cost. However, calorific value, in particular, can be determined through simpler methods by using ash and moisture values. The aim of this study was to develop a model that reduces the time and labor costs of coal companies by determining the calorific value and ash content of coal with the back-propagation algorithm of artificial neural networks (ANN). The model design was developed based on the data that was obtained from the laboratory analyses of raw coals from the pits of Tuncbilek and Seyitomer mining areas in Turkey. The values of moisture, volatile matter, original ash and sulfur were determined as input variables, and the lower calorific values and ash content were selected as output variables. The lower calorific values (LCV) and Ash estimated by the developed model were compared with the LCV obtained in the laboratory tests and the results showed a correlation. In addition, two different ANN models and multiple regression analysis (MRA) were developed to obtain the single output of the LCV and ash parameters with similar features. As a result, the ANN model and MRA equation models proposed in this study was shown to successfully estimate the LCV and ash content of coals without performing laboratory analyses.

Keywords: lignite chemical analyses, artificial neural networks, Seyitomer lignite, Tuncbilek lignite

1. Introduction

A major characteristic of developed countries is their high capacity of energy production. It is vital that the energy production of any country be higher than its energy consumption for the development of the industry and the increase of the national income. The high level of energy production depends on the most efficient utilization and use of energy production resources. Fossil fuels are a large part of energy production. Particularly due to the oil crisis in the 1970s, the use of coal as an alternative to oil, which meets most of the global energy production need, started to increase and the coal-related exploration and research boosted. Today, 30% of the world's energy is produced using coal. In addition, metallurgical coke produced from coking coal is used for 75% of the world's liquid pig iron production (Kural, 1998).

Artificial neural network prediction model is widely used in order to gain rapid results in the development of coal production technology or mining industry. Ambrozic and Turk (2003) showed that surface subsidence in Velenje Coal Mine fields could be successfully predicted using artificial neural networks. Similarly, Zhao and Chen (2011) successfully observed the change of surface sedimentation with respect to the time variation in metal mineral deposits using artificial neural networks. Yin et al. (2003) determined successful prediction models for coal blending by using various artificial neural networks and different training models. Chelgani et al. (2010) successfully used artificial neural

networks and multiple regression models to predict maximum reflectance and gross calorific value (GCV) of coal using volatile matter, carbon, total sulfur, hydrogen, and oxygen values. Feng et al. (2015) constructed the back-propagation neural network, decision support machine and alternating conditional expectation models for GCV estimation using 76 results from Chinese coal analysis. The back-propagation neural network model provides more consistent results in the training phase than the other models, while the alternating conditional expectation model is superior in the generalization phase. Zhou et al. (2017) showed that the ANFIS is highly accurate in the quantitative assessment of fault-induced water inrush. Allahkarami et al. (2017) showed the use of artificial neural network and multiple regression models to predict cobalt and nickel ions removal from wastewater.

Energy production is vital for Turkey as for the whole world. As a country that is rich in coal reserves, Turkey needs to improve the efficiency and technology of coal production. In this study, laboratory analyses of raw coals and other coals produced in all of the processes in Tuncbilek and Seyitomer pits were examined by using artificial neural networks (ANN) in order to minimize time and cost. The objective at this stage was to determine whether ANN back-propagation algorithm modeling could be used to predict the laboratory analysis values of moisture, volatile matter, original ash and sulfur content of coal without actually carrying out laboratory analyses for lower calorific value (LCV) and ash content. This study compares the LCV and ash content values estimated by the proposed model and the LCV and ash content values obtained in real laboratory settings.

2. Materials and methods

Garp Lignite Enterprise (GLE) extracts coal from both underground and open pits in Tuncbilek and neighboring areas. Samples are taken periodically or at random times from raw coal of underground and open pits of GLE and from drilled coal of Seyitomer Lignite pits. These samples are delivered to the laboratory branch office by sample technicians. The parameters that are used to determine the quality of lignite coal and preferred in this study are shown in Table 1. Moisture, volatile matter, ash, dry sulfur, original ash and LCV of the samples are determined by means of laboratory analyzers (Table 1). In this study, an ANN model was designed by using the results of 2500 sample analyzes obtained through the above-mentioned process. As separate sets, 2100, 390 and 400 pieces of data selected randomly from the total data set were divided into groups for training, test and data verification, respectively (Gulec, 2014). Using these data groups, three different models were created. First of all, an ANN model was developed using the double output variable within the same model. Then two different ANN models were developed under the same conditions but with output parameters used separately. Finally, models were constructed based on the equations obtained by using the MRA method.

Firstly, an independent variable importance analysis, which is a sensitivity analysis, was performed by using SPSS.16, assuming that the target is ash and LCV and the inputs are original ash, humidity, dry sulfur and volatile matter content. The sensitivity analysis determines how much the value predicted by the network model varies for different values of the independent variable. Normalized importance is basically the importance values divided by the largest importance values and expressed as percentages. As can be seen in Fig. 1 on the importance values of the output variables, the impact scores of original ash, which was the most effective parameter, moisture, volatile matter and dry sulfur were 0.512, 0.342, 0.131 and 0.015, respectively. For this reason, original ash, moisture, volatile matter and dry sulfur were used as inputs of the ANN application. In addition, whether our input parameters were orthogonal or not was tested using Pearson correlation analysis. As shown by the results in Table 2, the input parameters used in our study are not common variables.

The network model of the implemented ANN back-propagation algorithm is shown in Fig. 2. The model application was performed with software by using the original ash, moisture, volatile matter and sulfur contents as the inputs for ANN, and LCV and ash contents as output variables for ANN. The designed ANN consisted of feed-forward back propagation, two hidden layers, training function (Levenberg-Marquardt), adaptation learning function (Gradient descent learning function), transfer function (Hyperbolic Tangent Sigmoid Transfer Function) and performance function (MSE-mean squared error) as demonstrated in Figure 2. Momentum rate and learning rate values were determined and the model was trained through iterations. The parameter values obtained from C#-based ANN back-propagation algorithm were given in Table 3.

The ANN models were compared according to the absolute fraction of variance (R^2), mean absolute percentage error (MAPE) and a root-mean squared (RMS) error criteria. These criteria are defined by Eqs. (1), (2) and (3), respectively (Gulbandilar and Kocak, 2016).

$$RMS = \sqrt{\frac{1}{N} \sum_{i=1}^N |t_i - o_i|^2} \quad (1)$$

$$R^2 = 1 - \left(\frac{\sum_{i=1}^N (t_i - o_i)^2}{\sum_{i=1}^N (o_i)^2} \right) \quad (2)$$

$$MAPE = \frac{1}{N} \sum_{i=1}^N \left(\left| \frac{t_i - o_i}{o_i} \right| \right) * 100 \quad (3)$$

where t is the target value, o is the network output value, and N is the total number of pattern. In the training and testing of ANN model from experimental data and average of these test results are used.

Table 1. Statistical distribution of training data used to construct the ANN Model

Statistical parameters	Input variables				Output variables	
	Moisture (%)	Original Ash (Kg)	Sulfur (Kg)	Volatile Matter (Kg)	Ash (Kg)	LCV (kJ)
Mean	16.686	13.144	2.641	38.986	15.728	5.211
Std. Error of Mean	0.063	0.074	0.011	0.036	0.083	0.007
Std. Deviation	3.194	3.682	0.562	1.801	4.139	0.367
Minimum	6.25	5.97	1.31	18.76	7.32	3.979
Maximum	27.10	33.05	5.59	46.13	37.84	6.286

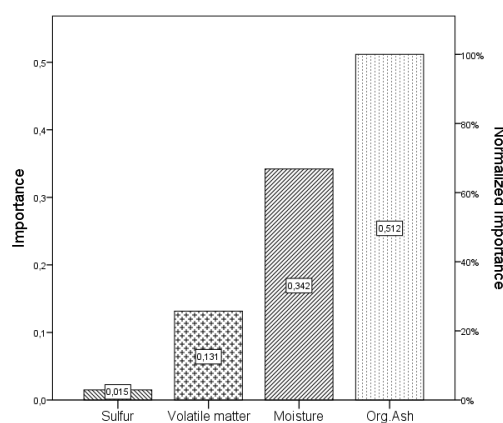


Fig. 1. Reliability analysis of raw coal laboratory results

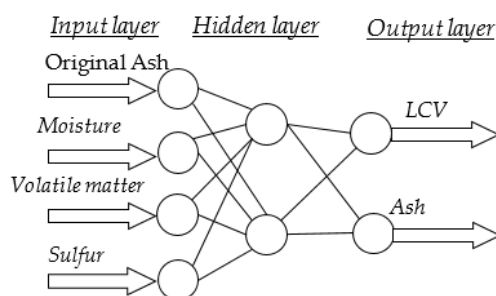


Fig. 2. Network model developed in application

Table 2. Orthogonality analysis results of input parameters

Input variables	Correlation coefficient
Moisture-Original ash	-0.304
Moisture-Sulfur	-0.275
Moisture-Volatile matter	0.294
Original ash- Sulfur	0.240
Original ash-Volatile matter	-0.714
Sulfur- Volatile matter	-0.075

Table 3. The values of parameters used in model

Parameters	Value
Number of input layer neurons	4
Number of hidden layer	2
Number of first hidden layer neurons	10
Number of second hidden layer neurons	2
Number of output layer neuron	2
Error after learning	1x10 ⁻⁴
Learning rate	0.9
Epoch	1000
Momentum rate	0.5

3. Results and discussion

After the execution of the ANN application, the process was terminated when the acceptable error value was reached in the training process. The real LCV of the raw coal were compared to the LCV resulting from the training of the ANN application (Fig. 3). There was a significant relationship between R^2 , MAPE and RMS values on the figure and the data. Also, the SPSS analyses performed on the training by using 2100 sets of data did not find any statistically significant difference ($C_{LCV}=1$, $C_{ash}=0.972$, $P<0.001$).

In order to determine the accuracy of our trained model, 400 randomly separated data sets were used for verification purposes. The LCV and ash values obtained from the test data and the experimental LCV and ash values were compared (Fig. 4 and Fig. 5). As can be seen in the scatter plot, there was a significant relationship among the data for R^2 , MAPE and RMS results. In addition, the analyses performed on the test data did not find any statistically significant difference ($C_{LCV}=0.998$, $C_{ash}=0.923$, $P<0.001$).

A total of 392 data samples randomly selected from the dataset for the trained ANN model were used to test the model. The LCV and ash values obtained from the test data and the experimental LCV and ash values were compared (Fig. 6 and Fig. 7). As can be seen in the scatter plot, there was a significant relationship among the data for R^2 , MAPE and RMS results. In addition, the analyses performed on the test data did not find any statistically significant difference ($C_{LCV}=0.973$, $C_{ash}=1$, $P<0.001$).

Taking LCV and ash value of raw coal as the target, a reliability analysis was performed in SPSS for moisture, volatile matter, original ash, and dry sulfur parameters. According to the importance values of the output parameters, the impact scores of original ash, moisture, volatile matter and dry sulfur were 0.512, 0.342, 0.131 and 0.015, respectively. The positive results obtained in the training and test results of the ANN, which was designed considering these levels of importance, confirm that our success was not accidental.

As mentioned above, the ANN application performed in C# software language, the original ash, moisture, dry sulfur and volatile matter contents of the raw coal were used as the input parameters. The ANN was trained using a total of 2100 data sets, verified with 400 data sets and tested with 392 data sets.

The regression analysis for the LCV and ash values of the raw coal obtained from the training of our ANN model and the real LCV and ash values obtained as a result of laboratory analyzes found $R^2 =$

0.9457 for the LCV and $R^2 = 0.999$ for ash. Also, the correlation value was found as $C=1$ for the LCV and $C=0.971$ for ash. Similar success was achieved during the ANN testing stage, too.

The ANN model with the same technical parameters mentioned above was repeated by constructing models for the single output parameters. The training results of the LCV of the first ANN model that was generated were evaluated. Comparison of the model's training results and the experimental results showed that the performance of the developed model was significantly higher than that of the developed model with $R^2 = 0.9545$, MAPE = 1.116 and RMS = 0.7196. A different ANN model with the same technical characteristics was developed for the second output variable, ash, and it was found that the training performance of this model also had a high learning ability ($R^2 = 0.9999$, MAPE = 0.0393 and RMS = 0.1834). In addition, two different equation models were obtained by MRA analysis using the same training data set. In order to determine the LCV variable, the first model was obtained using the mathematical equation:

$$LCV = 8637.113 - 109.277 * Moisture - 90.556 * Original Ash + 10.885 * Sulfur - 11.245 * Volatile matter$$

We could suggest that the obtained equation shows high performance in defining the data set ($R^2 = 0.999$, $p < 0.001$). Secondly, the MRA equation obtained

$$Ash = -2.847 + 0.195 * Moisture + 1.181 * Original Ash + 0.017 * sulfur - 0.006 * Volatile matter$$

could be used in defining ash content. This equation obtained for ash content also yielded successful results in defining the data set ($R^2 = 0.950$, $p < 0.001$). Therefore, the three different models developed using data sets collected from the fields in our study yielded very successful results in determining LCV and ash output parameters (Table 4).

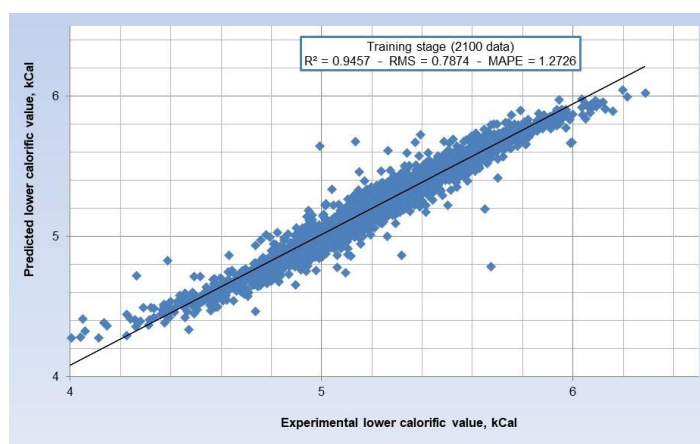


Fig. 3. Scatter plot of the LCV obtained as a result of the raw coal values used as training data and the experimental LCV

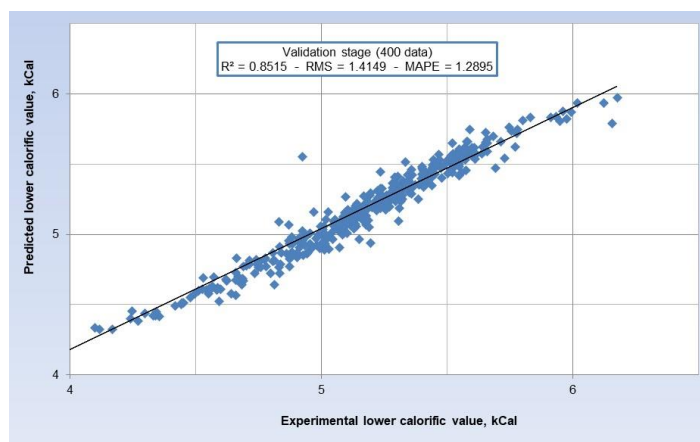


Fig. 4. Scatter plot of the LCV obtained as a result of the raw coal values used as validation data and the experimental LCV

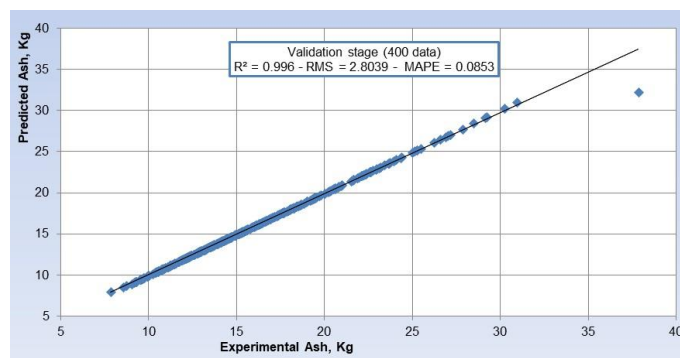


Fig. 5. Scatter plot of the real ash values obtained as a result of the raw coal values used as validation data and the experimental ash values

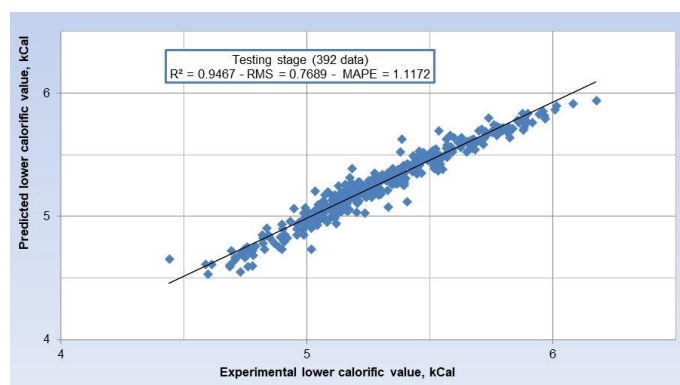


Fig. 6. Scatter plot of the LCV obtained as a result of the raw coal values used as test data and the experimental LCV

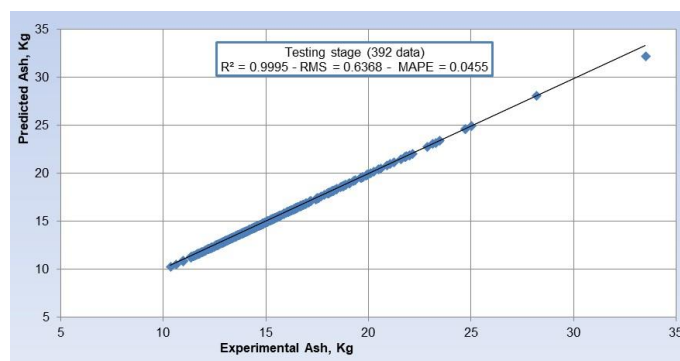


Fig. 7. Scatter plot of the real ash values obtained as a result of the raw coal values used as test data and the experimental ash values

Table 4. The total statistical results of the comparison of the achievements of the developed models (R^2)

Output variables	LCV			Ash		
	ANN-single	ANN-double	MRI	ANN-single	ANN-double	MRI
Training/ Calculating	0.9545	0.9457	0.9999	1	0.9999	0.95
Validation	0.959	0.8515	0.8826	0.996	0.996	0.9937
Test	0.943	0.9467	0.9931	0.9995	0.9995	0.998

4. Conclusions

The results showed that the performance of the proposed ANN models and MRA equations is very high and its use for coal analysis in the mining sector will be profitable in terms of labor cost and time. Data sets in the ANN model proposed and implemented in this study were obtained from certain regions

and certain types of coal. Use of data sets from more diversified coals can possibly increase the model's power and applicability by including different properties and analyzes of coal to the model in addition to the coal analysis values used.

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