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Estimation of coal proximate analysis factors and calorific value by multivariable regression method and adaptive neuro-fuzzy inference system (ANFIS)

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ABSTRACT

The proximate analysis is the most common form of coal evaluation that reveals the quality of a coal sample. It examines four factors including moisture, ash, volatile matter (VM), and fixed carbon (FC) within the coal sample. Every factor is determined through a distinctive experimental procedure under ASTM specified conditions. These determinations are time consuming and require various laboratory equipment. The calorific value is one of the most important properties of a solid fuel and its experimental determination requires special instrumentation and highly trained operator. This paper develops mathematical and ANFIS models for estimation of two factors of proximate analysis based on the other two factors. Furthermore, the estimation of calorific value of coal samples based on proximate analysis factors is performed using multivariable regression, the Minitab 16 software package, as well as ANFIS and MATLAB software package. The results indicate that ANFIS is a more powerful tool for estimation of proximate analysis factors and calorific value than multivariable regression method. The following equation estimates the calorific value of coal samples with high precision:
Calorific value (btu/lb)= 12204 - 170 Moisture + 46.8 FC - 127 Ash

Keywords : *Coal, Proximate analysis, Calorific value, Data modeling, Regression and ANFIS methods*

1. Introduction

Chemical composition of a coal sample is defined in terms of its proximate and ultimate (elemental) analyses [1,2]. The proximate analysis is performed in order to determine the moisture, ash, volatile material (VM) and fixed carbon (FC) content within the coal sample and is reported as a percentage of the weight of the coal sample used [1,2]. It is applied to establish the rank of coals, to show the ratio of combustible to incombustible constituents, or to provide the basis for many coal buying/selling and performance prediction indices used by utility operators [1,2]. Moisture, VM, and ash are all determined by subjecting the coal to preset temperatures for predetermined time intervals under ASTM specified conditions [1,2]. The losses of weight are, by stipulation, due to loss of moisture and, at the higher temperature, loss of VM. After recording these measurements, the tester burns the coal and the remaining material is called ash [1,2]. FC is the difference of these three amounts summed and subtracted from one hundred. In low volatile coal samples, the FC content is approximately equal to the elemental carbon content of the sample [1, 2]. These determinations, however, are time consuming and require various laboratory equipment. Therefore, it is very desirable to both the suppliers and consumers of coal to have an exact and reliable estimation method for obtaining the proximate analysis factors.

The calorific value is one of the most important characteristics of a fuel which defines its energy and is useful for planning and control of a combustion plant [3]. The experimental determination of calorific value of solid fuels is an expensive process, as it requires special instrumentation and highly trained operators. Therefore, to simplify the task and to reduce the cost of analysis, many correlations were developed for determining calorific value from proximate and ultimate analysis data of solid fuels, whereas these analytical data can be obtained more conveniently. Several researchers have used regression method to develop an equation between calorific value and proximate analysis factors (FC, Ash, VM and Moisture) or ultimate analysis factors (moisture, ash, carbon, hydrogen, nitrogen, sulfur, and oxygen) [4-8]. The developed models for estimation of calorific value or higher heating value (HHV) of solid fuels are summarized in Table 1.

Table 1. Proposed mathematical models for estimation of calorific value.

Equations	comments	Ref.
Q = 0.3278C + 1.419H+ 0.09257S - 0.1379O + 0.637 (MJ/kg)	C, H, S, and O are on a dry, mineral-matter free	[4]
Q = 0.472C + 1.48H + 0.193S+0.107Ash-12.29 (MJ/kg)	C, H and S all on dry basis	[5]
HHV = 35.43- 0.1835VM - 0.3543 Ash (MJ/kg)	VM and Ash on dry basis	[6]
HHV = -2737- 160.43 Moisture + 266.76 VM (MJ/kg)	as received sample	[7]
HHV = -0.03 Ash- 0.11Moisture + 0.33 VM + 0.35 FC (MJ/kg)	as received sample	[8]

Artificial neural network (ANN) is a computational-based, nonlinear empirical modeling tool, which is analogous to the behavior of

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biological neural structures [9, 10]. Krishnaiah et al. suggested a method to compute ultimate analysis based on the proximate analysis information using ANN [11]. Estimation of gross calorific value of coals using ANN has been performed by Patel et al. [12].

ANFIS is a specific approach in neuro-fuzzy which is a powerful tool for modeling the nonlinear functions [13]. The ANFIS can simulate and analyze the mapping relation between the input/output dataset through a back-propagation algorithm alone or in combination with a least mean squares method (hybrid learning) to optimize the parameters of a given Fuzzy Inference System (FIS) [14, 15].

The estimation of two factors of coal proximate analysis based on the other two factors has not received enough attention. In this paper we performed the estimation using multi-variable regression, the Minitab 16 software package, and the ANFIS MATLAB software package. In this research, we also tried to establish a model for estimation of calorific value based on proximate analysis factors. Hence, the best subsets regression by Minitab 16 software was applied for the first time to identify the model with as few variables as possible and then the model was developed by multivariable regression, the Minitab 16 software. An ANFIS model was also developed for estimation of calorific value with proximate analysis factors as variables by MATLAB software package and a comparison was made between these models.

2. Experimental data

A mathematical model needs a comprehensive database to cover a wide variety of coal types. Such a model will be capable for estimating the proximate analysis factors with a high accuracy. The results of proximate analysis of total 270 United States coal samples reported by U.S. bureau of mines [16] were used for the development of mathematical and ANFIS models. The Boxplot of proximate analysis factors and calorific value are illustrated in Fig.1. The dataset was randomly divided into two parts; training and testing dataset. The number of training and testing dataset was 249 and 21, respectively. The training dataset was used for establishment a mathematical model or the training ANFIS. In order to get more reliable evaluation and comparison, mathematical and ANFIS models are tested with testing dataset that was not used during the training process. The performance of mathematical models and ANFIS configurations was validated through calculating the average relative deviation (ARD%) which is defined as:

$$\mathrm{ARD\%} = \frac{\sum_{i=1}^{N} \left| \frac{(y_i^{exp} - y_i^{cal})}{y_i^{exp}} \right|}{N} \times 100 \qquad (1)$$

Where y_i^{exp} and y_i^{p} are experimental and calculated values for the i[th] dataset, and N is the total number of considered events.

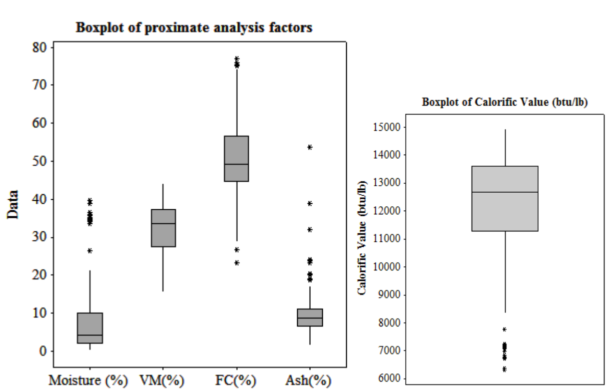

Fig. 1. Boxplot of proximate analysis factors and calorific value of 270 US coal samples.

3. Adaptive neuro-fuzzy inference system (ANFIS)

The concept of ANFIS algorithm was first introduced by J. Jang (1993) [17]. It combines the advantages of two intelligent approaches, neural network and fuzzy logic, to allow good reasoning in quantity and quality [18].

Like other fuzzy systems, the ANFIS structure is organized of two introductory and concluding parts which are linked together by a set of rules. A kind of this network, which is a first-order Takagi-Sugeno fuzzy model with two inputs and one output, is illustrated in Fig.2. As can be seen, this system contains two inputs namely *x* and *y* and one output or *f* which is associated with the following rules:

- Rule 1: If x is A_1 and y is B_1, then $f_1=p_1x+q_1y+r_1$;
- Rule 2: If x is A_2 and y is B_2, then $f_2=p_2x+q_2y+r_2$;

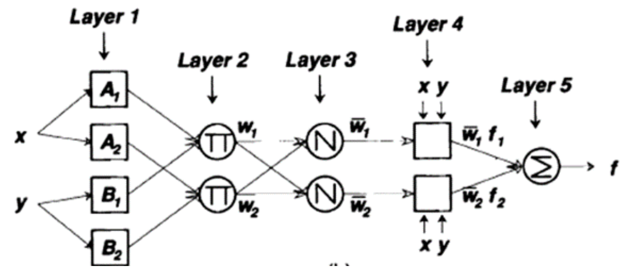

Fig. 2. ANFIS structure for a two-input Takagi-Sugeno model with two rules.

In this system, A_i, B_i and f_i are fuzzy sets and system's output, respectively. p_i, q_i and r_i are designing parameters which are achieved during the learning process. ANFIS is a multi-layer network and five distinct layers can be recognized in the structure of ANFIS network [18]. If we consider the output of each layer in the ANFIS network as $O_{i,j}$ (i^{th} node output in j^{th} layer), we may explain the various layers functions of this network as follows:

Layer 1: Every node *i* in this layer is an adaptive node with a node function

$$O_{1,i} = \mu_{A_i}(x), \quad \text{for} \quad i = 1,2 \quad \text{or} \qquad (2)$$
$$O_{1,i} = \mu_{B_{i-2}}(y), \quad \text{for} \quad i = 3,4$$

where *x* (or *y*) is the input to node *i* and A_i (or B_{i-2}) is a linguistic variable associated with this node function and μA_i is the membership function of A_i. The Gaussian membership function used in the ANFIS model is as follows:

$$\mu_{A_i}(x) = \exp\left(-\frac{(x-c_i)^2}{2a_i^{\,2}}\right) \qquad (3)$$

where x is input and {a_i, c_i} is the parameter set [13]. Parameters in this layer are referred to as premise parameters.

Layer 2: Every node in this layer is a fixed node labeled Π which calculates the firing strength w_i of a rule. The output of each node is the product of its all incoming signals and is given by:

$$O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y), \quad i = 1,2 \qquad (4)$$

Layer 3: Every node in this layer is a fixed node labeled N. The i^{th} node calculates the ratio of the i^{th} rule's firing strength to the sum of all rules' firing strengths:

$$O_{3,i} = \overline{w}_i = \frac{w_i}{w_1 + w_2}, \qquad i = 1,2. \qquad (5)$$

The output from the i[th] node is called the normalized firing strength.

Layer 4: Every node in this layer is an adaptive node with a node function given by

$$O_{4,i} = \overline{w}_i f_i = \overline{w}_i (p_i x + q_i y + r_i), \qquad i = 1,2 \qquad (6)$$

where $\overline{w}_i$ is a normalized firing strength from layer 3 and {p_i, q_i, r_i} is the consequent parameter set of this node.

Layer 5: The single node in this layer is a fixed node labeled ∑, which calculates the overall output as the summation of all incoming signals:

$$\text{overall output} = O_{5,i} = \sum_i \overline{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i}, \quad i = 1,2 \qquad (7)$$

4. Results and discussion

4.1. Regression analysis

4.1.1. Predication of proximate analysis factors

In order to develop correlations between one of the proximate analysis factors and the other two factors, a multivariable regression using least squares was performed by Minitab 16 software. Table 2 shows equations for estimation of FC and p-values of the models and the parameters. The P value for all three equations is 0.000 which indicates that the models estimated by the regression procedure are significant at an α-level of 0.05. The p-values for the estimated coefficients are both 0.000, indicating that they are significantly related to FC. Table 2 also shows the R^2 and ARD values for both of training and testing datasets. The ARD values further indicate that the models fit the data well. The best model for estimation of FC includes moisture and VM. It has the highest R^2 value (80.2%) and the lowest ARD value (7.42).

Table 2. Equations for estimation of FC and related R^2 and ARD values.

Equation	P value				R^2 (%)	ARD		Eq. No.
	Model	constant	1st variable	2nd variable		Train data	Test data	
FC = 68.5 - 1.08 Moisture - 0.951 Ash	0.000	0.000	0.000	0.000	64.3	11.08	10.75	Eq. (8)
FC = 94.1 - 0.813 Ash - 1.10 VM	0.000	0.000	0.000	0.000	54.6	12.54	7.29	Eq. (9)
FC = 89.1 - 0.918 Moisture - 0.972 VM	0.000	0.000	0.000	0.000	80.2	7.20	7.42	Eq. (10)

Fig.3 shows the normal plot of residual, histogram of residual, the residual versus fits plot and the residual versus order plot for estimation of FC through Eq.8. The points in normal probability plot generally form a straight line which indicates the distribution of residuals. The plot of residuals versus the fitted values shows that the residuals get greater as the fitted values increase, which may indicate that the residuals have non-constant variance. The residual versus order plot is a plot of all residuals in the order that the data was collected and can be used to find non-random error. It can be seen that there is non-random error since the points show a random pattern.

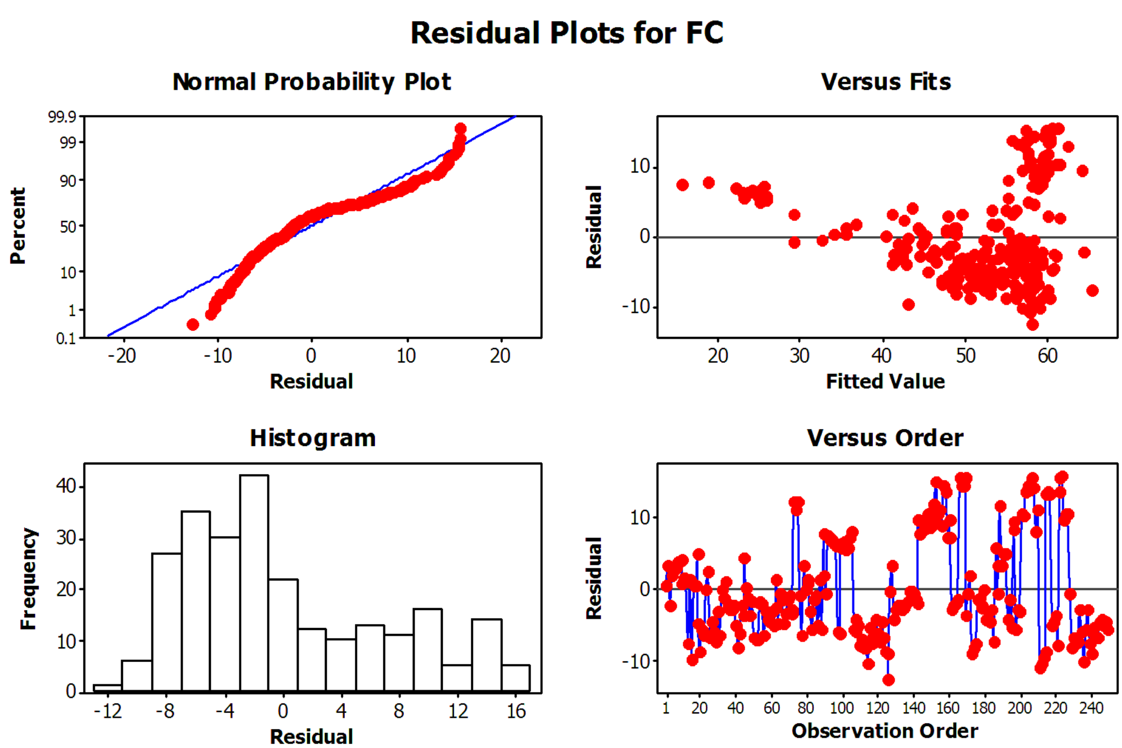

Fig.3. Residual plots for estimation of FC through Eq.8

Table 3 shows three different equations for estimation of VM. The p value for Eq. 11 is 0.290 which indicates that the model estimated by the regression procedure is not significant at an α-level of 0.05. The R^2 value for this equation is 1% which further indicates that the model is not appropriate for fitting the data. The p-value for Eq. 12 and Eq. 13 are both 0.000 which indicate that the models are significant at an α-level of 0.05. The p-values for estimated coefficients are both 0.000, indicating that they are significantly related to VM. Eq.13 is the best model for estimation of VM since it has the lowest ARD value for testing datasets (8.03).

Table 3. Equations for estimation of VM and related R^2 and ARD values

Predicted equation	p-value				R^2 (%)	ARD		Eq. No.
	Model	constant	1st variable	2nd variable		Train data	Test data	
VM = 31.5 + 0.0782 Moisture - 0.0488 Ash	0.290	0.000	0.167	0.570	1	22.00	15.77	Eq. (11)
VM = 69.2 - 0.566 Moisture - 0.649 FC	0.000	0.000	0.000	0.000	63.4	10.22	9.07	Eq. (12)
VM = 58.4 - 0.395 Ash - 0.445 FC	0.000	0.000	0.000	0.000	49	13.57	8.03	Eq. (13)

Three different equations for estimation of Ash are presented in Table 4. The P value for Eq. 14 is 0.115 which reveals that the model estimated by the regression procedure is not significant at an α-level of 0.05. The p-value for Eq. 15 and Eq. 16 are both 0.000 which indicate that the models are significant at an α-level of 0.05. The ARD value for both equations is high which indicates that the accuracy of the models for the estimation of Ash is not satisfactory. Eq.16 is the best model for estimation of Ash since it has the lowest ARD value (52.06) for testing datasets.

Table 4. Equations for estimation of Ash and related R^2 and ARD values

Predicted equation	p-value				R^2 (%)	ARD		Eq. No.
	Model	constant	1st variable	2nd variable		Train data	Test data	
Ash = 10.9 - 0.0812 Moisture - 0.0270 VM	0.115	0.000	0.053	0.570	1.7	43.05	71.71	Eq. (14)
Ash = 30.8 - 0.434 Moisture - 0.351 FC	0.000	0.000	0.000	0.000	34.5	42.43	68.79	Eq. (15)
Ash = 34.4 - 0.278 FC - 0.333 VM	0.000	0.000	0.000	0.000	22.8	39.68	52.06	Eq. (16)

4.1.2. Predication of calorific value

The best subsets regression is an efficient way to identify models with as few variables as possible which achieve our goals. Subset models may actually estimate the regression coefficients and predict probable responses with smaller variance than the full model using all variables [19, 20]. Minitab examines all possible subsets of the predictors, beginning with all models containing one variable, and then all models containing two variables, and so on. By default, Minitab displays the two best models for each number of variables. A good model should have a high R^2 and adjusted R^2, small S, and a Mallows' Cp close to the number of variables in the model and the constant [19, 20].

The results of best subsets regression by Minitab software are presented in Table 5. Each row of the Table 5 represents a different model. Vars is the number ofpredictor variables in the model. Variables that are present in the model are indicated by an x.

Table 5. The results of best subsets regression by Minitab software for estimation of calorific value

Vars	R^2	R^2 (adj)	Mallows Cp	S	Variables type			
					Moisture	VM	FC	Ash
1	76.7	76.6	1397.7	935.23			x	
1	72.4	72.3	1700.1	1017.7	x			
2	95.5	95.4	76.2	413.12		x	x	
2	93.7	93.6	202.4	487.98	x			x
3	96.5	96.5	3.1	361.95	x		x	x
3	96.5	96.5	3.2	362.07	x	x	x	
4	96.5	96.5	5	362.65	x	x	x	x

The three-predictor model with all variables except VM has the highest R^2 and adjusted R^2 (96.5%), the lowest Mallows' Cp value (3.1) and S value (361.95). The model with all the variables has the highest R^2 and adjusted R^2 values (96.5%), a low Mallows' Cp value (5) and S value (362.65). The best two-predictor model includes VM and FC, with a higher Cp value (76.2) and a lower adjusted R^2 (95.5%). The best one-predictor models might be considered the minimum fit.

The best model to predict the calorific value is a three-predictor model with all variables except VM as following equation:

$$\text{Calorific value (btu/lb)} = 12204 - 170\ \text{Moisture} + 46.8\ \text{FC} - 127\ \text{Ash} \quad (17)$$

The p value for the model is 0.000 which indicates that the models estimated by the regression procedure are significant at an a-level of 0.05. The p-values for all of the estimated coefficients are 0.000, indicating that they are significantly related to calorific value. The R^2 value for this equation is 96.5% which indicates that the model fit the data well. The ARD value for training and testing datasets were 2.18 and 14.99%, respectively.

4.2. FIS estimation

4.2.1. Estimation of proximate analysis factors

In this research, a hybrid grid partitioning ANFIS by using Gaussian membership function was developed in order to predict two factors of coal proximate analysis based on the other two factors. An ANFIS toolbox from MATLAB is used and its operation is explained in its user guide.

For estimation of FC content of coal samples by ANFIS, six different schemes are possible. In three schemes, the estimation of FC is performed directly through ANFIS modeling. In other schemes, the estimation of FC is carried out indirectly by applying this fact that the summation of moisture, ash, FC and VM content of coal samples is 100 percent. Table 6 shows different schemes for the estimation of FC content of coal samples. As can be seen, the ARD value for estimating the FC content of coal samples in scheme 3 has the least value among the other schemes. In this scheme, moisture and VM content are input parameters in ANFIS modeling and FC content is output parameter.

Table 6: Different schemes for estimation of FC content of coal samples and the related ARD values.

Scheme No.	Input Parameters		Output Parameter	ARD		Calculated Parameter	
				TEST	TRAIN	Name	ARD
1	Moisture	Ash	FC	7.06	7.35	VM	10.26
2	Ash	VM	FC	8.99	9.18	Moisture	102.52
3	Moisture	VM	FC	6.43	6.05	Ash	61.8
4	Moisture	VM	Ash	61.68	34.96	FC	6.56
5	Ash	VM	Moisture	89.33	109	FC	7.05
6	Moisture	Ash	VM	10.69	15.46	FC	7.17

Fig.4 shows the applicability of ANFIS modeling for the estimation of FC through scheme 3. As can be seen, this scheme has a good ability for estimation of FC content of coal samples. Fig.4 also compares the ability of regression method and ANFIS for estimation of FC content of coal samples. As can be seen, ANFIS can show better results in estimation of FC than regression method.

The estimation of VM content of coal samples by ANFIS is possible through six different schemes. In three schemes, the estimation of VM is performed directly through ANFIS modeling and in other three schemes the estimation of VM is carried out indirectly, as explained previously. Table 7 shows different schemes for the estimation of VM content of coal samples. Scheme 8 is the best schemes for the estimation of VM since it has the lowest ARD value (4.59%).

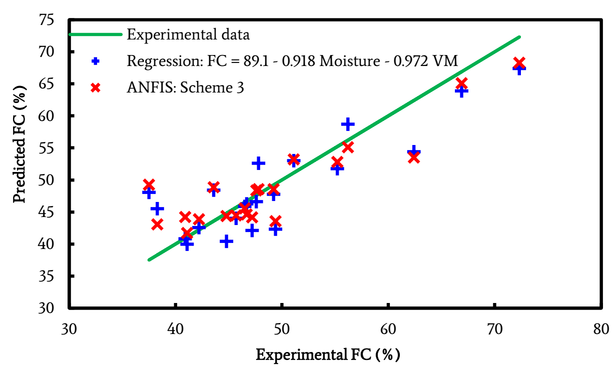

Fig.4. The plot of experimental FC content of coal samples versus predicted FC by regression method and ANFIS

Table 7: Different schemes for estimation of VM content of coal samples and the related ARD values.

Scheme No.	Input Parameters		Output Parameter	ARD		Calculated Parameter	
				TEST	TRAIN	Name	ARD
6	Moisture	Ash	VM	10.69	15.46	FC	7.17
7	Moisture	FC	VM	6.88	6.24	Ash	52.02
8	Ash	FC	VM	4.59	4.99	Moisture	46.35
1	Moisture	Ash	FC	7.06	7.35	VM	10.26
9	Moisture	FC	Ash	53.05	28.47	VM	7.26
10	Ash	FC	Moisture	42.85	43.40	VM	4.60

Fig.5 shows the applicability of ANFIS modeling for the estimation of VM content of coal samples through scheme 8. It can be seen that this scheme has a good ability for estimation of VM content of coal samples. Fig.5 plots a comparison between ANFIS and regression method for estimation of VM. The results indicate that ANFIS is a better predictor for VM than regression method.

The estimation of ash content of coal samples by ANFIS was performed similar to the estimation of FC and VM and the results presented in Table 8. The lowest ARD value for the estimation of ash content of coal samples is observed for scheme 11.

The applicability of ANFIS modeling for the estimation of ash content of coal samples through scheme 11 is illustrated in Fig.6. It can be seen that it presents good performance in estimation of ash content of coal samples. Fig.6 also compares two methods of regression and ANFIS for estimation of Ash content of coal samples. The figure confirms that ANFIS is a better method for estimation of Ash than regression method.

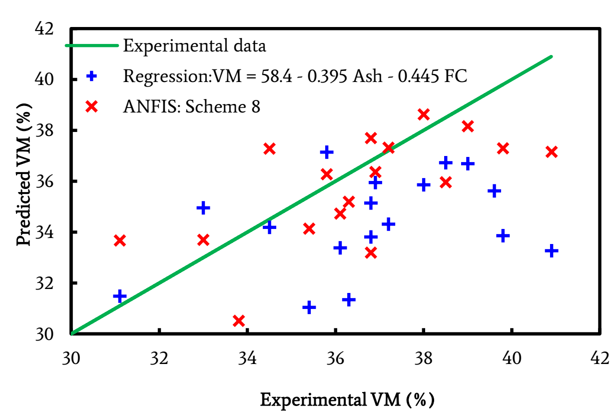

Fig.5. The plot of experimental VM content of coal samples versus predicted VM by regression method and ANFIS.

Table 8. Different schemes for estimation of ash content of coal samples and the related ARD values.

Scheme No.	Input Parameters		Output Parameter	ARE		Calculated Parameter	
				TEST	TRAIN	Name	ARE
4	VM	Moisture	Ash	61.68	34.96	FC	6.56
9	Moisture	FC	Ash	53.05	28.47	VM	7.26
11	VM	FC	Ash	36.02	31.05	Moisture	42.65
3	Moisture	VM	FC	6.43	6.05	Ash	61.8
7	Moisture	FC	VM	6.88	6.24	Ash	52.02
12	VM	FC	Moisture	53.39	68.89	Ash	43.38

The applicability of ANFIS modeling for the estimation of ash content of coal samples through scheme 11 is illustrated in Fig.6. It can be seen that it presents good performance in estimation of ash content of coal samples. Fig.6 also compares two methods of regression and ANFIS for estimation of Ash content of coal samples. The figure confirms that ANFIS is a better method for estimation of Ash than regression method.

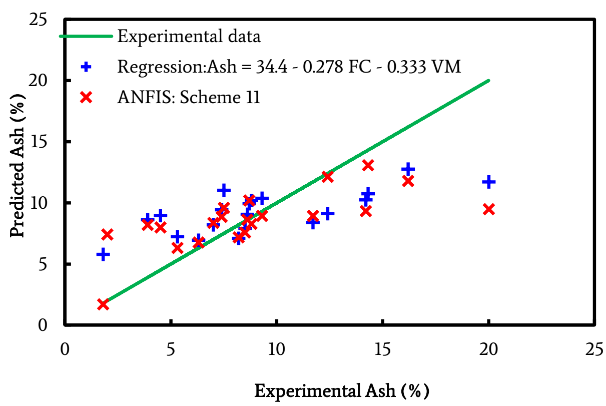

Fig.6. The plot of experimental Ash content of coal samples versus predicted Ash by regression method and ANFIS.

4.2.2. Estimation of calorific value

Based on grid partitioning algorithm by Gaussian Membership Function with proximate analysis factors (i.e., Moisture, VM, FC and Ash), ANFIS model was designed to predict calorific value (Fig.7).

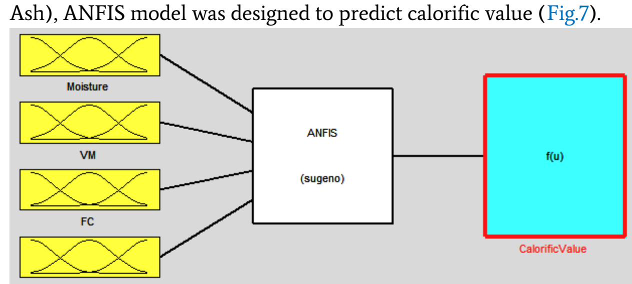

Fig. 7. System ANFIS: 3 inputs (Moisture, VM, FC and Ash), 1 output (Calorific Value)

Fig.8 shows the ANFIS model structure that was built for calorific value estimation in this study. Also, the characterizations of ANFIS models are shown in Table 9.

The ARD value for training and testing datasets was 2.85% and 3.07%, respectively. These values indicate that the developed model by ANFIS for estimation of calorific value is accurate and consistent. Fig.9 shows the applicability of ANFIS model to predict calorific value based on proximate analysis factors. As can be seen, ANFIS model maintains its excellent estimation accuracy throughout the range of calorific value, hence showing consistency and a high degree of generalization capability. A comparison between regression method and ANFIS for estimation of calorific value has been also shown in Fig.9. It can be seen that the ANFIS model could predict the calorific value more precisely than the regression model.

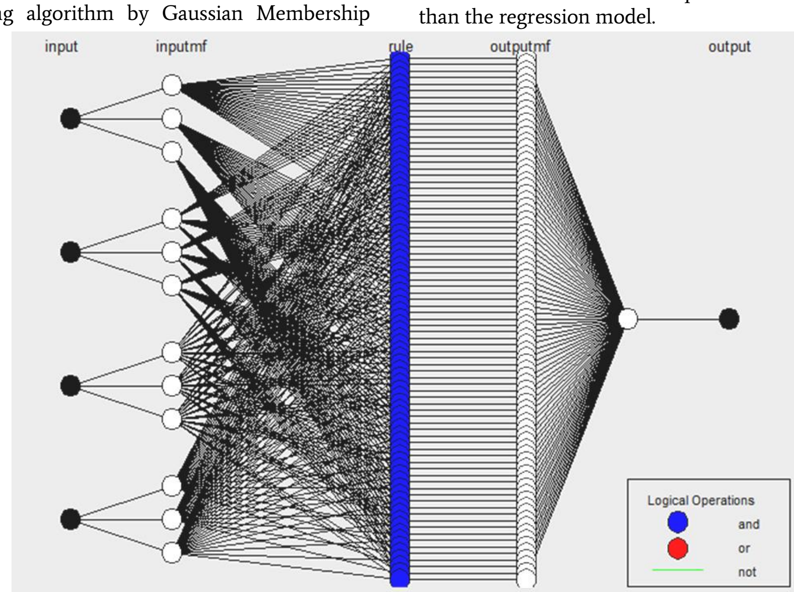

Fig.8. Model structure of the ANFIS for calorific value estimation.

Table 9. Summary of the ANFIS model structures and optimal parameters.

ANFIS parameter type	Value
Number of MFs	3 3 3 3
Output MF	Linear
Number of nods	193
Number of linear parameters	81
Number of nonlinear parameters	48
Total number of parameters	129
Number of training data pairs	249
Number of testing data pairs	21
Number of fuzzy rules	81
Number of epoch	2000

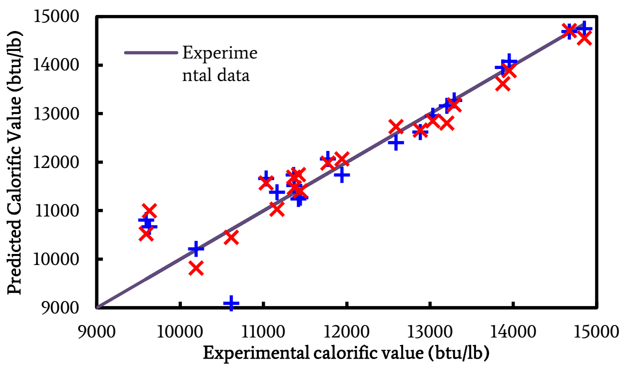

Fig.9. The plot of experimental calorific value versus predicted calorific value by regression method and ANFIS.

5. Conclusion

The mathematical and ANFIS models were developed for estimation of two factors of proximate analysis based on the other two factors. The best mathematical models for estimation of FC, VM and Ash with multiple regression method by Minitab 16 software were found to be as follows:

FC = 89.1 - 0.918 Moisture - 0.972 VM

VM = 58.4 - 0.395 Ash - 0.445 FC

Ash = 34.4 - 0.278 FC - 0.333 VM

The best input variables for estimation by ANFIS for FC were Moisture & VM, for VM were Ash & FC, and for Ash content of coal samples were FC & VM. The results indicated that ANFIS is a more powerful tool for estimating the proximate analysis factors than multivariable regression method.

Different set of the proximate analysis factors were evaluated with the best subsets regression by Minitab16 software to find the best mathematical model for estimating the calorific value. The results showed that the three-predictor model with all variables except VM had the highest R^2 and adjusted R^2 (96.5%), the lowest Mallows' Cp value (3.1) and S value (361.95). The model had shown fairly small deviations when applied to a diversity of coal samples, thus providing a rapid, convenient and cost effective procedure to obtain good estimates of calorific value. The ability of ANFIS was also examined for estimating the calorific value of coal samples from proximate analysis factors. The results indicated that the accuracy of ANFIS for estimation of calorific value is better than that of regression method.

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