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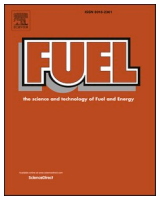

Full Length Article

Estimation of the coal higher heating value for energy systems relied on ultimate analysis with machine learning techniques

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ABSTRACT

The calorific value of solid fuels, also referred to as the gross calorific value (GCV) or the higher heating value (HHV), is a crucial property for its use as a fuel in energy systems. The HHV of coal as a resource can be predicted by more effective algorithms that use schedule information in engineering, like *ultimate analysis*, enabling fast decisions about its use as fuel in energy systems. The goal of this research was to acquire a global artificial prediction model relied on an interesting algorithm, a nonlinear model termed multivariate adaptive regression splines (MARS), in addition to the grid search (GS) optimizer, for characterization of coal HHV (output variable) using constituents of coal ultimate analysis: carbon (C), nitrogen (N), oxygen (O), hydrogen (H) and sulphur (S) (5 specific input variables). Moreover, a multivariate linear regression (MLR) and a multilayer perceptron-type (MLP) artificial neural network (ANN) were adjusted to the observed data as well as known empirical correlations for comparison purposes. The current investigation has produced two results. The MARS model is used to first demonstrate the significance (or strength) of each input variable on the coal HHV (output variable). Second, the most accurate predictor of the coal HHV was the MARS–relied approximation. In fact, using this method on coal testing samples resulted in a MARS regression with coefficients of determination and correlation coefficients for the coal HHV estimation of 0.9921 and 0.9960, respectively. The agreement between the data that were observed and those that were predicted using the GS/MARS–relied approximation proved that the latter had performed satisfactorily.

1. Introduction

Coal is one of the primary solid fuel most used and analyzed in the world for energy production [1,2]. Coal has a high carbon content and varying concentrations of other elements, primarily hydrogen, sulphur, oxygen, and nitrogen. During the Carboniferous and Cretaceous periods were formed most of the coal that is currently being mined. The decomposition of terrestrial plants as biomass that accumulate in shallow marshes, lagoons, or oceanic areas gives rise to coal. Progressive carbon enrichment occurs over time. Later, they could be covered with deposits of clay, which would help maintain the anaerobic conditions necessary for the carbonization process to continue from biomass [3,4].

There are numerous varieties of coal, which can be classified according to characteristics such as: (1) moisture; (2) percentage in non-combustible mineral matter (ash); (3) the heating power; and (4) flammability, in connection with the percentage of volatile elements. Ultimate analysis is a chemical test that provides the mass fraction of each of the five elements that primarily make up all types of coal: carbon (C), nitrogen (N), oxygen (O), hydrogen (H) and sulphur (S).

Due to the various types of plants from which they originate and, more importantly, the duration and circumstances (i.e., pressure and temperature of the carbonization process), there are four different types of coal, which are (see Fig. 1):

- Peat: the most recent coal is this one. It is light in weight, soft, matte, and brown with visible plant remnants.
- Lignite: it is dark-colored. It is a soft coal that dates (like peat) from periods after the Carboniferous, so the carbonization process has not completely taken place. It has a brittle shine and the appearance of burnt wood.
- Bituminous coal: It is a tough, fully carbonized coal that is glossy black in color (from pearly gloss to bright and matte bands).
- Anthracite: It is a hard coal (very compact and bright) with a pearlescent shine and a black color that is completely carbonized.

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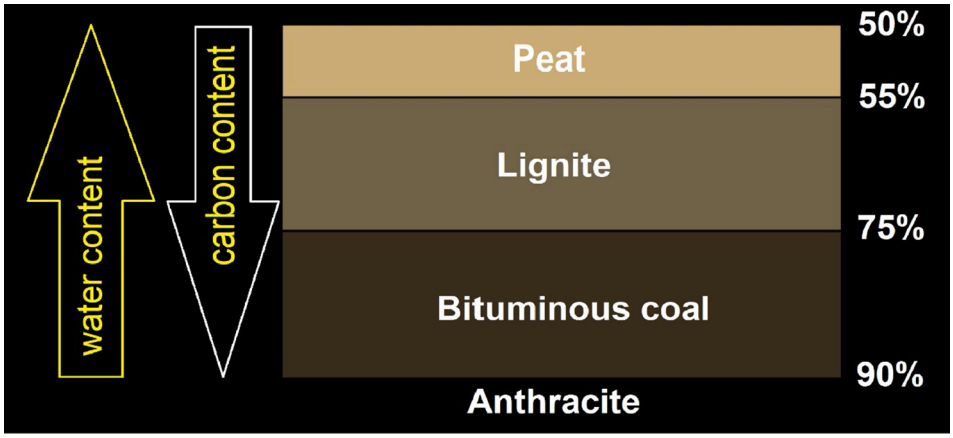

Fig. 1. Main types of coal.

Coal is the most used and widely dispersed type of fossil fuel in the world, from resource to energy, which is a chemical storage of solar energy [3,5]. Coal-related businesses make a principal contribution to international trade. This fossil fuel is commercially extracted in more than 50 countries and is used industrially in more than 70 countries. Indeed, the world's annual consumption of coal is approximately 5.8 billion tons. The generation of electrical energy in thermal power plants consumes 75% of this world production. Due to the growing demand for energy, the amount of coal consumed is likely to roughly double by 2030 [6].

The calorific value of coal determines its energy, so knowing the precise calorific value of coal is important for distinct requirements such as: (1) its classification; (2) the precise determination of its energy potential; (3) encountering an area of productive use; and (4) its exact value in the commodity market. Furthermore, the coal's heating value is a critical factor in the correct design and appropriate operation of coal-fired devices [7]. Experimental measurement of HHV from coal through the required devices is pricey and time consuming [8]. Therefore, obtaining and implementing a technique that allows the precise and rapid determination of HHV in coal would be highly desirable and would imply considerable savings compared to experimental tests in the laboratory. To fix ideas, there are several previous investigations in the literature that build mathematical empirical correlations for the coal HHV foretelling from the elemental constituents of ultimate analyses [9–14]. However, new models to foretell the coal HHV are being developed using statistical machine learning techniques (MLT) in the last decade, which may be more accurate than the aforementioned empirical correlations and which also contribute to saving the costs of the usual experimental tests.

Making tools and software that can carry out tasks that ordinarily require human intelligence is the focus of the broad field of study known as artificial intelligence. In this way, a subset of artificial intelligence known as machine learning (ML) uses algorithms to discover patterns and draw conclusions from data [6–8]. Making techniques for computer learning is the aim of machine learning. When an agent's performance improves over time and with the aid of data, this is when learning is said to have occurred. In machine learning, data is analyzed by a computer, a model is built from the data, and the model is then employed as a world hypothesis and a tool to solve problems. The development and implementation of algorithms based on artificial intelligence (i.e. machine learning) represent significant advances in tackling multiparametric analysis for energy conversion through modeling engineering. The algorithms and models are designed to identify patterns in data, learn from those patterns, and then use what they have learned to make predictions or take actions [7,8].

Statistical machine learning-based prediction models have been used in the coal-related literature studies. Examples of such previous research coal HHV prediction models relied on statistical machine learning are known in the published literature and they include the use of the decision tree regression [15], adaptive neurofuzzy inference system [16], a multilayer perceptron jointly with genetic algorithms [17], and Gaussian process regression [18]. However, it has not yet been investigated whether multivariate adaptive regression splines (MARS) can be used to forecast coal's higher heating value (coal HHV).

Ultimate analysis is a technique utilized to identify the elemental composition of coal, typically including carbon, hydrogen, oxygen, nitrogen and sulphur [10–12]. The data obtained from the elemental analysis of coal is critical to determine its chemical composition, and subsequently predict its characteristics, such as heating value and suitability for practical applications. This information is also vital in evaluating the potential of energy conversion and environmental impact of coal by combustion, as it can assist in identifying the levels of greenhouse gas emissions and other pollutants [11,12].

In general, understanding the characteristics and behavior of coal as a fuel depends heavily on ultimate analysis. This method requires burning a sample of the coal in an oxygen-rich environment, causing the elements in the sample to convert to their oxide forms. The resulting gases are then separated and analyzed using gas chromatography or mass spectrometry. In this way, the analytical procedure relies on the complete and instantaneous oxidation of the sample, which converts all compounds to combustion products. The resulting gases could then be selectively separated in a chromatographic column as a base procedure before being transported using a carrier gas through a reduction tube. Finally, a thermal conductivity detector that generates a signal proportional to the concentration of each individual component in the mixture could be used to process the separated gases (see Fig. 2).

Fig. 2 shows a flowchart of the procedure of coal ultimate analysis:

Fig. 2. Illustrative process diagram of the experimental procedure.

1. Coal sampling: A representative sample of coal to be analyzed is taken. The sample is dried, pulverized, and sieved to obtain fine and homogeneous particles.
2. Combustion: The sample is burned in a high-temperature furnace in an oxygen-rich atmosphere to convert the elements present in the sample into their corresponding oxides. The resulting gases are then transported through a reduction tube using a carrier gas, such as helium, and separated in a chromatographic column.
3. Detection: The separated gases are then passed through a thermal conductivity detector, which produces a signal based on the relative amounts of each component in the mixture.
4. Data analysis: The analysis results are used to determine the elemental composition of the coal and can be used to predict its properties and suitability for different applications.

To the authors' knowledge, the relevance of this method, which estimates the coal HHV from observed coal samples using the multivariate adaptive regression splines (MARS) approximation [19–24] and the optimizer known as Grid Search (GS) [25–28], has not been intended to be put before research at this time. In order to estimate the coal HHV output variable for the comparison purposes, a multivariate linear regression (MLR) [29–33] and a multilayer perceptron-type (MLP) [8,17,19,25] artificial neural network (ANN) were also fitted to the observed dataset. With the ability to handle nonlinearities and the presence of factor interactions, MARS is a nonparametric approximation that can be used to solve regression problems [19–24].

Preceding investigations have shown that MARS is a useful tool in many different fields, including informatics, medicine, and engineering [34–37]. Undoubtedly, the following are a few justifications for the usefulness of the proposed MARS approximation [20–24]: (1) compared to linear regression strategies, MARS approximations are easier to implement; (2) the same set of basis functions always comes out when the same initial dataset is used as the MARS approximation's input; (3) it is fairly easy to comprehend and understand MARS approximations; (4) both categorical and continuous data can be handled by MARS; and (5) MARS approximations offer an explicit mathematical expression of the output dependent factor as a function of the input factors through the summation of basis functions (that is, hinge functions and products of two or more hinge functions). Because the majority of ML techniques function effectively like a black box, this last characteristic just mentioned is a critical distinction from other ML techniques (multilayer perceptron, etc.).

The principal goal of the present study is to assess the use of various ML techniques to foretell the coal HHV from the chemical input factors of the ultimate analysis of various coal samples. These techniques include an optimised GS/MARS–relied model, a MLR–type approximation and a MLP-type approach. In order to successfully evaluate the coal HHV dependent variable, it has been investigated the actions of five input constituents, specifically carbon (C), nitrogen (N), oxygen (O), hydrogen (H), and sulphur (S) (see Fig. 2).

The following is the order in which this original investigation is set up. First, the necessary tools and procedures for performing this investigation are specified. The results are presented and discussed in the second step. Next, the key conclusions derived from the results are then presented.

2. Materials and methods

The equation created by Dulong or the use of a bomb calorimeter are currently the two most widely used techniques for determining the heating value of fuels [38]. In this way, based on empirical modeling and using experimental data from the composition of solid fuels (coal in our case), such as proximate or ultimate analyses, a number of mathematical equations and models have been developed [39]. To facilitate energy research based on statistical machine learning, more sophisticated models for fuels could be applied in this research environment.

Table 1
The coal physico-chemical input and output parameters employed in this study jointly with their means and standard deviations as well as their minimum and maximum values.

Input variables	Name of the parameter	Mean	Standard deviation	Minimum value	Maximum value
Carbon content (wt%)	C	78.64	2.73	72.72	83.72
Hydrogen content (wt%)	H	5.02	0.26	4.71	5.71
Oxygen content (wt%)	O	13.03	2.51	8.60	17.64
Nitrogen content (wt%)	N	1.30	0.16	0.99	1.63
Sulfur content (wt%)	S	1.70	0.51	0.53	2.52
Output variable					
Coal higher heating value (MJ/kg)	HHV	30.92	1.63	26.50	34.63

Note: wt% means *weight percentage*.

2.1. Experimental dataset

The experimental ultimate analyses and their related higher heating values (HHVs) make up the coal dataset used in this investigation. The dataset employed for both the GS/MARS-based, MLR-based and MLP-based approaches is based on a few physico-chemical parameters. The data used in this study were obtained from laboratory analysis, based on previous studies in the field of ultimate analysis of coal [40], where a total selection of 318 values were processed consisting of 318 samples of coal and five variables: carbon content (C), oxygen content (O), hydrogen content (H), nitrogen content (N), sulphur content (S), and higher heating value (HHV) (see Appendix A). The ultimate analysis of coal has selected the key input factors for this study. Heating value of coals is a key property for the iron industry and efficiency of the coal-fired power plants. Advanced models based on statistical machine learning are necessary for evaluating energy performance and identifying feasible alternatives for fuels to aid researchers in solid fuel characterization and management in an energy context [13,41–44].

When coal is used as a fuel for thermal applications, it is essential to calculate its heating value [45]. The heating value (HV), also known as the higher heating value (HHV), determines how much energy a fuel contains in a specific process. The maximum possible heat potential of a solid fuel is indicated by the HHV, which is typically expressed as a unit of energy per mass, frequently on a dry weight basis. Using an adiabatic bomb calorimeter to experimentally estimate HHV is expensive and not always practical [46]. Additionally, the ultimate analusis of coal can be an alternative to evaluate its physical and chemical properties. The weight percentages of carbon (C), oxygen (O), hydrogen (H), nitrogen (N), and sulphur (S) can all be calculated using elemental analysis [47].

A fuel's comprehensive analysis and higher heating value give a thorough understanding of its combustion properties. To define and describe in detail the behavior of a specific coal as fuel, these parameters are required. Consequently, the model's input variables are as follows on a dry basis (see Table 1):

- Ultimate analysis:
- Carbon (C): It is a portion of carbon that makes up the solid fuel's atomic structure.
- Hydrogen (H): Hydrogen content of the coal identified through elemental analysis.

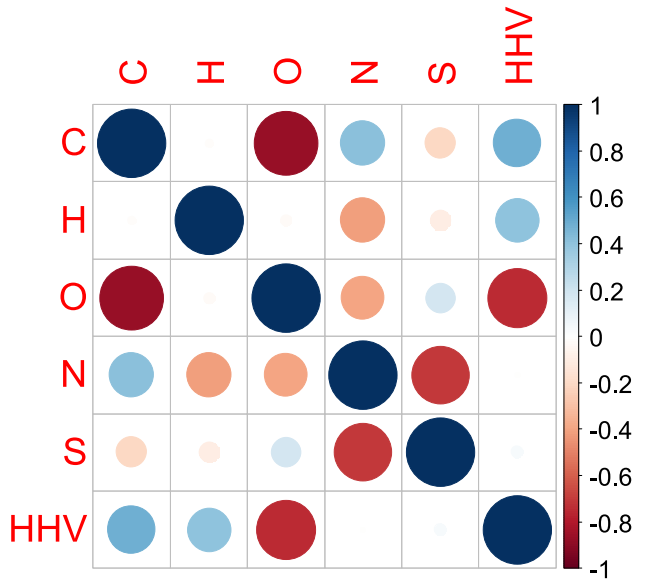

Fig. 3. Correlation matrix of the process variables: carbon content (C), hydrogen content (H), oxygen content (O), nitrogen content (N), sulphur content (S) and higher heating value (HHV) of coal.

- Nitrogen (N): It is a portion of nitrogen that makes up the solid fuel's atomic structure.
- Oxygen (O): Oxygen content of the coal identified through elemental analysis.
- Sulphur (S): Sulphur content of the coal identified through elemental analysis.

Table 1 contains a list of the five independent physico-chemical input factors to the GS/MARS model. Additionally, the coal higher heating value (coal HHV) attained from samples of various types of coal is the dependent variable in this investigation.

As an initial data analysis, a correlation matrix is calculated for all the variables that take part in the process. Fig. 3 shows graphically how close the two variables are on having a linear relationship with each other. Each variable in the table is correlated with each of the other variables. This allows us to see which pairs have the highest correlation.

2.2. Multivariate adaptive regression splines (MARS) method

The flexible nonparametric method known as multivariate adaptive regression splines (MARS) [19–25] enables the solution of regression problems. This approach generalizes both SL (*stepwise linear*) regression and CART decision trees [25,48] while overcoming their limits. Its main objective is to predict the values of a pleiad of independent input variables,$\boldsymbol{X}(n \times p)$, for a continuous output (dependent) variable $\boldsymbol{y}(n \times 1)$. The following expression describes the MARS method [19–25]:

$$\boldsymbol{y} = f(\boldsymbol{X}) + \boldsymbol{e} \tag{1}$$

Here:

- f: it consists of a sum of basis functions that depend on $\boldsymbol{X}$, weighted together and;
- $\boldsymbol{e}$: it is the $(n \times 1)-$ dimensional error vector.

The dependent variable and independent variables do not need to have an established functional relationship prior to using the MARS methodology. In a specific way, it can be expressed mathematically by a collection of piecewise polynomials of degree q (basis functions), where the coefficients are completely deduced from the whole regression $(\boldsymbol{X},\boldsymbol{y})$. The MARS method is developed by fitting different intervals of the

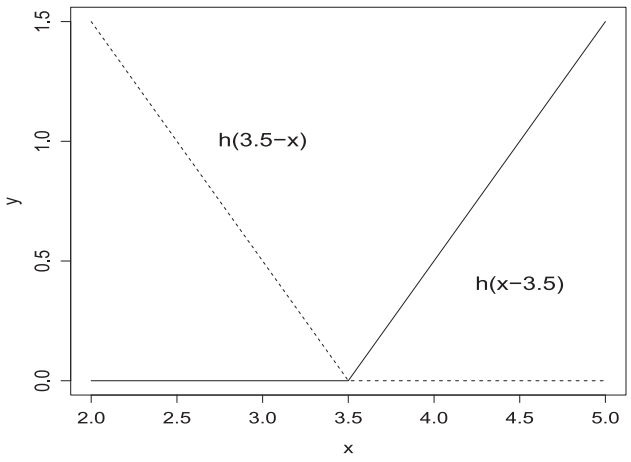

Fig. 4. Illustration of two linear hinge functions (also known as spline basis functions). The left spline $(x < t, -(x-t))$ is indicated by a dashed line, while the right spline $(x > t, +(x-t))$ is illustrated by the solid line.

independent variables with basis functions. Undoubtedly, two-sided truncated power functions are the basis functions employed as splines in MARS. Their expressions are as follows [19–25]:

$$[-(x-t)]_+^q = \begin{cases} (t-x)^q & if\ x < t \\ 0 & otherwise \end{cases} \tag{2}$$

$$[+(x-t)]_+^q = \begin{cases} (t-x)^q & if\ x \geq t \\ 0 & otherwise \end{cases} \tag{3}$$

so that the degree of flatness of the resulting function estimate depends on the power $q\ (\geq 0)$, which also determines the type of splines (linear, quadratic, or cubic). In this regard, if $q = 1$ conforms to linear splines (the area of this research), if $q = 2$ we have quadratic splines, if $q = 3$ cubic splines and so on. As an illustration, Fig. 4 displays two splines in case of $q = 1$ located at the node (or knot) $t = 3.5$.

As a result, the MARS approximation is a set of M basis function–based piecewise linear multivariate splines of a dependent variable that satisfy the following expression [19–25]:

$$\widehat{\boldsymbol{y}} = \widehat{f}_M(\boldsymbol{x}) = c_0 + \sum_{m=1}^{M} c_m B_m(\boldsymbol{x}) \tag{4}$$

Eq. (4) states the following:

- $\widehat{y}$: it is the output (dependent) variable foretold employing the MARS technique;
- c_0: is a constant factor (or coefficient) known as the *intercept*;
- $B_m(\boldsymbol{x})$: it is the m-th basis function; and
- c_m: it is the $B_m(\boldsymbol{x})$ basis function's corresponding coefficient.

Moreover, MARS employs generalized cross-validation (GCV) to ascertain the basis functions that comprise the complete approximation [19–25]. Undoubtedly, the *GCV* is established as the number resulting from division between the mean squared residual error and a penalization element. The penalty term is directly related to the complexity of the model. The *GCV* is expressed mathematically as follows [19–25,34–37]:

$$GCV(M) = \frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{f}_M(\boldsymbol{x}_i))^2}{(1 - C(M)/n)^2} \tag{5}$$

so that:

- The complexity penalization term $C(M)$ rises as the MARS model's number of basis functions does. This factor has the form [19–25,34–37]:

$$C(M) = (M+1) + d\,M \tag{6}$$

In a manner such that:

- M represents the number of basis functions in Eq. (5); and
- d is a penalty parameter defined by the model for each basis function.

For the purpose of producing reliable results, the factors N-subsets (this criterion indicates the number of subsets of the model in which each variable is integrated) and RSS (residual sum of squares) must be used in addition to the GCV factor previously mentioned [19–25,34–37].

2.3. Multivariate linear regression (MLR)

Multivariate linear regression (MLR) is a mathematical technique employed to build an approximate dependency relationship between a dependent variable Y, m independent variables X_i with $m \in Z^+$ and a random term ε (stochastic error) [29–33]. This method is applicable in many situations in which the relationship between two or more variables is studied or behavior is predicted. In case a regression model cannot be applied to a study, it is said that there is no correlation between the variables studied. This MLR model can be expressed as the following hyperplane of parameters β_i (called the coefficients of the multiple regression model) [29–33]:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_m X_m + \varepsilon = \beta_0 + \sum_{j=1}^{m} \beta_j X_j + \varepsilon \tag{7}$$

where:

- Y is the dependent variable or response variable;
- $X_1, X_2, \ldots, X_m$ are the m independent and explanatory regressor variables;
- $\beta_0, \beta_1, \beta_2, \ldots, \beta_m$ serve as the MLR model's parameters and gauge the explanatory variables' impact on the regressor. The number of independent parameters to take into account in the regression is indicated by the term m, while the terms β_0 and β_i $(i \geq 1)$ are the *intercept* and constant terms, respectively, for each independent variable.

The regression problem consists of choosing certain values for the unknown parameters β_j, so that the equation is completely specified. This requires a set of observations or a sample from this model. In any i-th observation (with $i = 1, 2, \ldots, m$), the simultaneous behavior of the dependent variable and the explicit variables is recorded (random disturbances are assumed to be unobservable). Suppose that we have a sample of size n given by $\{(x_{ij}, y_i)\}$ with $j = 1, 2, \ldots, m$ where x_{ij} denotes the i-th observed value in the regressor X_j and y_i denotes the i-th observation of Y, then the model takes the form [29–33]:

$$\widehat{y}_i = \beta_0 + \sum_{j=1}^{m} \beta_j x_{ij} + \varepsilon_i \tag{8}$$

where $\widehat{y}_i$ is the value of Y predicted by the MLR model, $\varepsilon_i = y_i - \widehat{y}_i$ is the error associated with the i-th measurement of the value X_j and follows the usual assumptions so that $\varepsilon_i \sim N(0, \sigma^2)$ (zero mean, constant variance and equal to σ^2, and $Cov(\varepsilon_i, \varepsilon_j) = 0$ if $i \neq j$). To assess the model parameters, the method of least squares can be used, in this case, the squared error function is given by [29–33]:

$$S(\beta_0, \beta_1, \ldots, \beta_m) = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{m} \beta_j x_{ij} \right)^2 \tag{9}$$

which we want to minimize. The least squares estimators denoted by β_0, $\beta_1, \beta_2, \ldots, \beta_m$ must satisfy [29–33]:

$$\left. \frac{\partial S}{\partial \beta_j} \right| = 0\,, \quad \forall j = 0, 1, 2, \ldots, m \tag{10}$$

This system with $m+1$ equations can be written in matrix form as [29–33]:

$$\boldsymbol{Y} = \boldsymbol{X\beta} + \boldsymbol{\varepsilon} \tag{11}$$

where $\boldsymbol{Y} \in \Re^{n\times 1}$, $\boldsymbol{X} \in \Re^{n\times(m+1)}$, $\boldsymbol{\beta} \in \Re^{(m+1)\times 1}$ and $\boldsymbol{\varepsilon} \in \Re^{n\times 1}$. In matrix form, the squared error function S can be written as [29–33]:

$$S(\boldsymbol{\beta}) = \sum_{i=1}^{n} \varepsilon_i^2 = \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} = (\boldsymbol{Y} - \boldsymbol{X\beta})^T (\boldsymbol{Y} - \boldsymbol{X\beta}) \tag{12}$$

and Eq. (10) is reduced to the *normal equations* [29–33]:

$$\boldsymbol{X}^T \boldsymbol{X} \widehat{\boldsymbol{\beta}} = \boldsymbol{X}^T \boldsymbol{Y} \tag{13}$$

Then, the least squares estimator is given by [29–33]:

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{Y} \tag{14}$$

So the final fitted multivariate linear regression model is given by [29–33]:

$$\widehat{\boldsymbol{y}} = \boldsymbol{X}^T \widehat{\boldsymbol{\beta}} = \widehat{\beta}_0 + \sum_{j=1}^{m} \widehat{\beta}_j x_j \tag{15}$$

2.4. Artificial neural network: Multilayer perceptron (MLP)

The third machine learning technique employed in this paper for coal HHV estimation is the artificial neural network (ANN) termed *multilayer perceptron* (MLP). ANN is a processing algorithm modelled on the neural structure of the human brain. Neurons are computational units that can be used to determine relationships and patterns between inputs and outputs [17,19,25]. The MLP is an artificial neural network (ANN) comprising numerous layers, so that it has the capacity to find a solution to nonlinearly separable problems, which is the principal restriction of the simple perceptron. The MLP has three types of layers [17,19,25,42]:

- Input layer: composed of those neurons that insert the input instances in the artificial neural network. These types of neurons do not undergo any mathematical processing.
- Hidden layers: composed of those neurons such that the inputs come from earlier layers and outputs are introduced to neurons from posterior layers.
- Output layer: composed of neurons such that the output values conform to their outputs of the complete artificial neural network.

Input nodes, that are part of the input layer, are connected with other nodes, the next layer, etcetera, up to reach the last layer, the output layer, which generates the hypothesis function. Hidden layers are composed of intermediate nodes located between input and output layers. The input characteristics are entered on the first layer (called the input layer). The intermediate nodes of the hidden layers use activation units to carry out some processing, using a matrix of weights, which direct the mapping from one layer j to the next layer $j+1$. What makes MLP distinct is the nonlinear *activation function* (AF), performed by the specific neural networks activation units [19,25,42]. Backward propagation (also known as backward propagation of the error or *generalised*

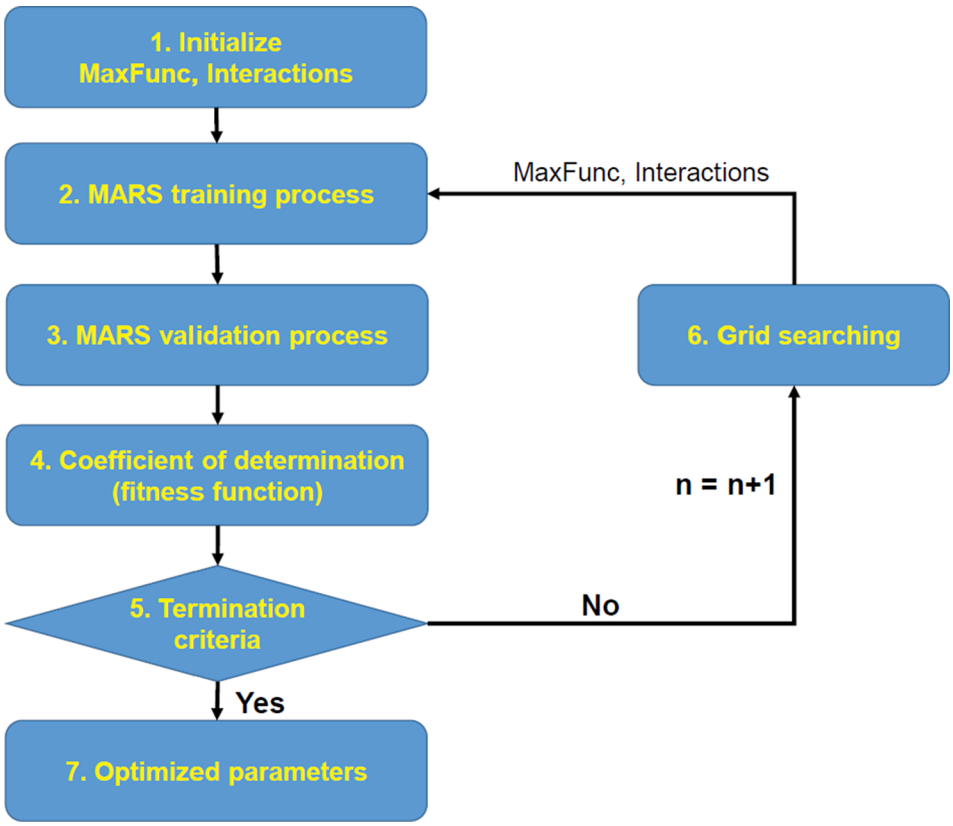

Fig. 5. The GS/MARS–relied approximation's process diagram.

delta rule) is an algorithm used in the training of these artificial neural networks. For this reason, the multilayer perceptron is also known as a backpropagation artificial neural network. The function implemented by the network is $f : X \subset \Re^n \rightarrow Y \subset \Re^c$, represented as [17,25,42]:

$$f(\mathbf{x}) \tag{16}$$

so that U represents the hidden variables space. Considering this architecture [17,25,42], we have that:

- $\psi_j(x) = \psi(w_j^T x + w_{j0})$: ψ represents the hidden layer AF; $w_j \in \Re^n$*is* a parameter; and $w_{j0} \in \Re$ is a threshold value. There are three types of AF: known as sigmoid, hyperbolic tangent and logistic AF, respectively.
- $\phi_j(u) = \phi(c_j^T u + c_{j0})$: ϕ is the AF of the neurons that make up the hidden layer; $c_j \in \Re^h$ are the weights; and $c_{j0} \in \Re$ is the threshold. Generally, ϕ is the dichotomous function (or Heaviside function).

To conclude, the MLP leads to the next function given by [17,25,42]:

$$f(\mathbf{x}) = \sum_{j=1}^{h} c_j \psi\left(\mathbf{w}_j^T \mathbf{x} + w_{j0}\right) + c_0 \tag{17}$$

2.5. The goodness–of–fit of this approach

The coefficient of determination R^2 is the primary goodness–of–fit statistic for the regression issue posed in this article [49,50]. It takes into account the following expressions if t_i and y_i, respectively, are the observed and predicted values [49,50]:

- $SS_{reg} = \sum_{i=1}^{n} (y_i - \bar{t})^2$: is the explained sum of squares.
- $SS_{tot} = \sum_{i=1}^{n} (t_i - \bar{t})^2$: the sample variance is directly correlated with this summation.
- $SS_{err} = \sum_{i=1}^{n} (t_i - y_i)^2$: it *is* termed as residual sum of squares.

so that $\bar{t}$ is the average value of the experimental data given by:

$$\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t_i \tag{18}$$

The coefficient of determination is then defined by the expression [49,50]:

$$R^2 \equiv 1 - \frac{SS_{err}}{SS_{tot}} \tag{19}$$

The discrepancy between experimental and predicted data gets smaller the closer the R^2 statistic is to 1.0. Similarly, the mathematical expressions for the other statistic used in this study (*RMSE*) is as follows [49,50]:

$$RMSE \equiv \sqrt{\frac{1}{n} \sum_{i=1}^{n} (t_i - y_i)^2} \tag{20}$$

Higher values of R^2 are preferred, i.e. closer to 1 means better model performance and regression line fits the data well. Conversely, the lower the *RMSE* value is, the better the model performs.

Moreover, the following hyperparameters are intensely employed in the MARS technique [19–25]:

- Maximum number of basis functions (Maxfuncs): at the conclusion of the forward phase, it corresponds to the maximum number of terms.
- Interactions: It reflects the strongest level of factor interaction.
- Penalty parameter (d): It is equivalent to the Generalized Cross Validation (*GCV*) penalty per node (or knot) that is associated with

Table 2
Intervals of variation of the two parameters of the GS/MARS–based approach fitted in this research.

MARS hyperparameters	Lower limit	Upper limit
Maximum number of basis functions (MaxFuncs)	3	100
Interactions	1	4

Table 3
The best–fitted GS/MARS approximation's optimal hyperparameters for the coal higher heating value (HHV) prediction.

Hyperparameters	Optimal values
MaxFuncs	18
Interactions	2

the complexity of the MARS approximation in Eq. (5). Be aware that terms are penalized if $d = 0$, but not nodes. Of course, there is no penalty if $d = -1$; the most common value of this parameter is $d = 2$.

In order to successfully optimize its estimation using the coefficient of determination R^2, various approximations have been built, specifically the MARS–relied approach, the MLR–type approximation and MLP-type approach in this study. These approximations take the coal HHV as a dependent factor from the five other factors (input variables) of experimental coal samples [40].

Additionally, as previously mentioned, the MARS approximation heavily depends on the MARS hyperparameters: maximum number of hinge functions (Maxfuncs); and ultimately, the degree of variable interaction. Grid search (GS), also known as *parameter sweeping* [25–28], is the common method of implementing hyperparameter optimization. It is simply a thorough manual search through a predetermined subset of the parameter space using that statistical machine learning algorithm.

In fact, the dataset is split into two sets: 80% of the data are used in the training set, and the remaining 20% are used in the testing set. In this way, the training collection is used to build the GS/MARS model. It uses a 10-fold cross-validation method to calibrate the parameters of the MARS model using the GS algorithm for this purpose [51,52]. When the optimal parameters were identified, the complete training dataset was used to build the model. Following that, it goes on to make predictions for the components of the testing set using this model. These predictions are contrasted with the observed values, and the model's goodness-of-fit is assessed. The process diagram for the GS/MARS–relied approximation used in this investigation is now illustrated in Fig. 5.

Additionally, cross-validation is also frequently used in this context to find the true coefficient of determination (R^2) [49,50]. Undoubtedly, a total 10-fold cross-validation method was employed in this investigation in order to evaluate the predictive capacity of the GS/MARS–relied approximation [51,52]. To achieve this, regression modeling using the MARS approximation has been implemented using the earth package from the R project [53,54]. Table 2 illustrates the variation intervals of the solution space used in this study.

For the purpose of optimizing the MARS parameters, the GS optimizer is appropriate. In this sense, the GS is able to determine the optimal Maxfuncs and Interactions parameters by means of the evaluation of differences of the cross-validation mistake in every iteration. The variation space is two-dimensional (one dimension per each parameter). Besides, in this investigation, the root mean square error (RMSE) serves as the objective function or principal fitness factor [49,50].

Table 4
Enumeration of hinge functions and its coefficients c_i of the best–fitted GS/MARS–relied approach for the coal HHV prediction.

B_i	Definition	c_i
B_1	1	28.2331
B_2	$h(82.8032 - C)$	−0.8113
B_3	$h(C - 82.8032)$	−0.7817
B_4	$h(16.6561 - O)$	1.3316
B_5	$h(O - 16.6561)$	−1.2716
B_6	$h(1.0816 - S)$	6.3654
B_7	$h(82.8032 - C) \times h(N - 1.4157)$	−10.6495
B_8	$h(82.8032 - C) \times h(1.4157 - N)$	2.3591
B_9	$h(82.8032 - C) \times h(N - 1.1681)$	3.8865
B_{10}	$h(82.8032 - C) \times h(S - 2.2016)$	0.9884
B_{11}	$h(82.8032 - C) \times h(2.2016 - S)$	0.4329
B_{12}	$h(5.357 - H) \times h(16.6561 - O)$	−0.8697
B_{13}	$h(H - 5.357) \times h(16.6561 - O)$	0.4725
B_{14}	$h(16.6561 - O) \times h(N - 1.2975)$	5.6533
B_{15}	$h(16.6561 - O) \times h(1.2975 - N)$	0.9829
B_{16}	$h(16.6561 - O) \times h(2.3062 - S)$	−1.2755
B_{17}	$h(1.1787 - N) \times h(S - 1.0816)$	−10.3962
B_{18}	$h(N - 1.1787) \times h(S - 1.0816)$	−6.5343

3. Results and discussion

Table 3 lists the optimal hyperparameters for the coal HHV's fitted MARS–relied approximation as determined by the GS optimizer.

Table 4 lists the principal basis functions and their coefficients c_i for the best–fitted GS/MARS-relied approximation for the coal HHV. Keep in mind that a hinge function is given by the expression:

$$h(x) = \begin{cases} x & \text{if} \quad x > 0 \\ 0 & \text{if} \quad x \leq 0 \end{cases} \tag{19}$$

Overall, the MARS technique is a type of nonparametric regression approach and can be considered as a generalization of linear methods. It uses a weighted summation of the *hinge functions* described above to automatically model the presence of nonlinearities as well as interactions between input variables [19–24].

Additionally, and in contrast, a multivariate linear regression (MLR) model and a multilayer perceptron (MLP) model have also been fitted to the observed dataset together with several empirical correlations [9–14] related to the coal HHV output factor too.

Next, Fig. 6 illustrates the first-order and second-order terms of the GS/MARS approach. This chart permits the understanding of the relationships among the distinct input variables entailed in this approximation. Using the previous chart, Coal higher heating value (Coal HHV) (Y-axis) as a function of Carbon content (X-axis) is represented in Fig. 6 (a), holding constant the four remaining input factors. In similar way, Fig. 6(b) and 6(c) show the Coal HHV (Y-axis) as a function of Oxygen content (X-axis) and Sulphur content (X-axis), holding constant the leftover four input variables, respectively. On the other hand, Fig. 6(d) illustrate the coal HHV (Z-axis) versus Carbon content (X-axis) and Nitrogen content (Y-axis), while the other variables remain constant. Analogously, Fig. 6(e-i) illustrate the coal HHV (Z-axis) as a function of the Carbon (X-axis) and Sulphur (Y-axis) contents, Hydrogen (X-axis) and Oxygen (Y-axis) contents, Oxygen (X-axis) and Nitrogen (Y-axis) contents, Oxygen (X-axis) and Sulphur (Y-axis) contents, and Nitrogen (X-axis) and Sulphur (Y-axis) contents, respectively.

The coal higher heating value (HHV) according to the MLR-type model based on the constituents of ultimate analysis (in mass percentage) is given by:

$$\mathrm{HHV(MJ/kg)} = -0.35\,.\,\mathrm{C} + 3.38\,.\,\mathrm{H} - 0.67\,.\,\mathrm{O} + 3.35\,.\,\mathrm{N} + 1.12\,.\,\mathrm{S} + 43.93 \tag{20}$$

Table 5 exposes some of the most used empirical formulas in the literature to determine the coal higher heating value (HHV), also based on the constituents of ultimate analysis in mass percentage. It seems

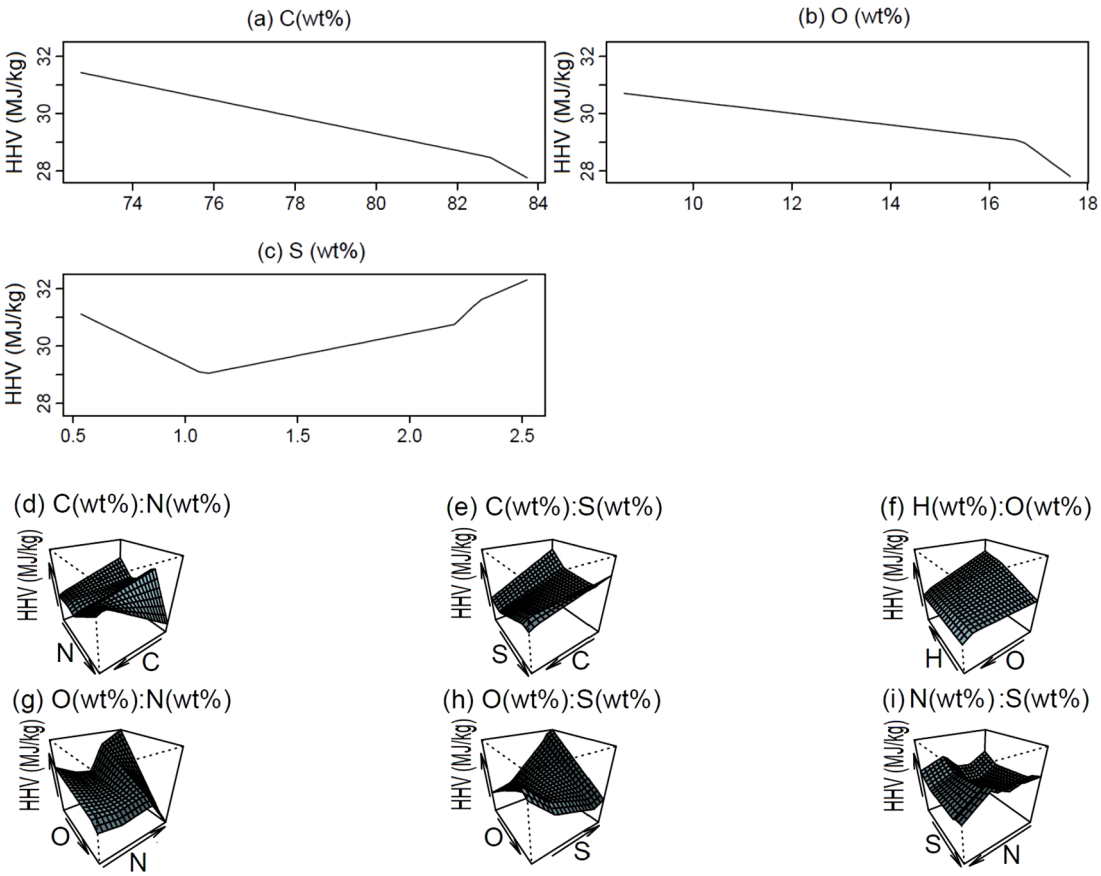

Fig. 6. Graphical drawing of the first-order and second-order terms that form the GS/MARS approximation for the Coal HHV: (a) Carbon content first-order term; (b) Oxygen content first-order term; (c) Sulphur content first-order term; (d) Carbon content and Nitrogen content term of the second order; (e) Carbon content and Sulphur content term of the second order; (f) Hydrogen content and Oxygen content term of the second order; (g) Oxygen content and Nitrogen content term of the second order; (h) Oxygen content and Sulphur content term of the second order; and (i) Nitrogen content and Sulphur content term of the second order.

Table 5
Coal HHV prediction empirical correlations based on the constituents of ultimate analysis [9–14].

Authors	Model equation
Channiwala and Parikh (2002) [9]	HHV(MJ/kg)=(1.0632 + 1.486•10^{-3})•[(C/3) + H•(O–S)/8] (E1)
Channiwala and Parikh (2002) [9]	HHV(MJ/kg) = 0.3403•C + 1.2432•H-0.0628•N–0.0984•O + 0.1909•S (E2)
Channiwala and Parikh (2002) [9]	HHV(MJ/kg)=(0.0152•H + 0.9875)•[(C/3) + H–O– (S/8)] (E3)
Channiwala and Parikh (2002) [9]	HHV(MJ/kg) = 0.3391•C + 1.4357•H+0.0931•S–0.1237•O (E4)
Mason and Gandhi (1983) [10]; Selvig and Wilson (1945) [11]	HHV(MJ/kg) = 0.336•C + 1.418•H–(0.153–0.00072•O)•O + 0.0941•S (E5)
Given et al. (1986) [12]	HHV(MJ/kg) = 0.336•C + 1.418•H-0.145•O + 0.0941•S (E6)
Chelgani (2021) [13]	HHV(MJ/kg) = − 0.110 + 0.385•C (E7)
Matin and Chelgani (2016) [14]	HHV(MJ/kg) = − 4.542 + 0.431•C + 0.283•S + 0.367•H + 0.645•N (E8)

Note: Specific ranges of validation for C, H, O, N and S are 0.00–92.25, 0.43–25.15, 0.00–50.00, 0.00–5.60 and 0.00–94.08, respectively, based on Ref. [2,9–14].

Table 6
Coefficients of determination (R^2), correlation coefficients (r) and root-mean-square errors (RMSE) for the GS/MARS–based approximation, MLP approach and MLR approach fitted in conjunction with several empirical correlations [9–14] fitted in this investigation to the coal HHV variable applied to the testing data.

Model	R^2	*r*	*RMSE*
GS/MARS	**0.9921**	**0.9960**	**0.1626**
MLP	0.9345	0.9667	0.3669
MLR	0.8683	0.9319	0.6926
E1	0.3633	0.6028	4.9905
E2	0.3955	0.6288	1.6737
E3	0.5025	0.7089	11.8547
E4	0.4119	0.6418	1.9688
E5	0.4158	0.6449	1.6044
E6	0.4209	0.6488	1.5915
E7	0.1682	0.4101	1.9189
E8	0.2032	0.4508	2.1738

important to indicate that the selected models for comparison are of general use in the bibliography for solid fuels characterization and model validation. Particularly, it has to mention Channiwala's and Parikh's works, which obtain a general equation for fuels [2].

Table 6 gives the determination and correlation coefficients for the GS/MARS–relied approximation, MLR-type model, MLP-type model and empirical correlations [9–14] for the coal HHV output factor applied to the testing data, each in order.

The best–fitted MARS approximation has a coefficient of determination R^2 of 0.9921 and a correlation coefficient of 0.9960 for the coal

Table 7
Input variables' order of relevance in the best–fitted GS/MARS–based approach for the coal HHV as stated in criterion *GCV*.

Input variable	Nsubsets	*GCV*	*RSS*
Carbon content (C)	15	100.0	100.0
Oxygen content (O)	14	16.8	21.3
Hydrogen content (H)	13	6.3	11.4
Sulphur content (S)	12	1.9	7.8
Nitrogen content (N)	10	1.7	7.3

HHV factor, each in order, as stated in these most recent statistical estimates, choosing this best model for estimating the dependent variable (coal HHV factor) in various types of coal. Thus, these outcomes show a reliable goodness–of–fit, or an appropriate agreement between the experimental data and MARS approximation.

As an additional result of these estimations, Table 7 and Fig. 7 show, each in order, the relevance order for the five input factors predicting the coal HHV (output dependent factor) in the form of a Pareto chart [49,50] for this complex research. Hence, as stated in the MARS model, the input variable carbon content (C) is the most important variable in predicting the coal HHV output variable, followed by oxygen content (O), hydrogen content (H), sulphur content (S), and nitrogen content (N).

The use of solid fuels as the coal requires knowledge of their base composition, i.e. ultimate analysis, and their thermal features, i.e. HHV. Ultimate analysis reveals the percentage of carbon (C), hydrogen (H), oxygen (O), nitrogen (N), and sulphur (S). Traditionally, (C), (H), and (O) can be used to determine HHV, while (N) and (S) provide a reference of the limitations of the energy management due to environmental impact and fuel conversion [55]. According to the ranking order in the GS/MARS-relied approximation, (C) is the primary element in the list for reporting HHV in the proposed model due to its direct contribution to the release of energy during combustion. The next elements in the ranking are (O) and (H) for measuring combustion characteristics and fuel quality. The significance of (C) and (H) for solid fuel was emphasized by Dulong, who proposed a models linking these variables [38]. (N) is the least important input variable. However, its effect of the last

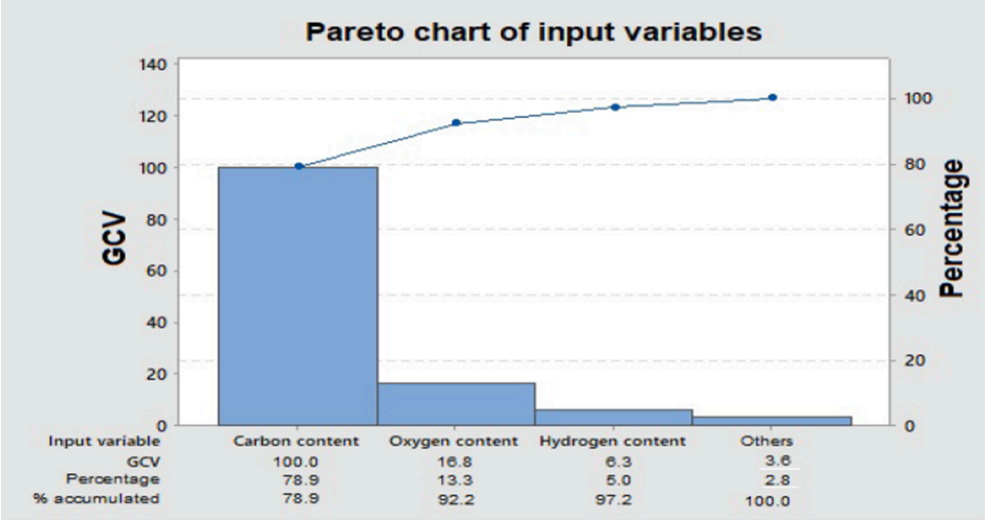

Fig. 7. Pareto chart of input variables: order of relevance for the input variables employed in the best–fitted GS/MARS–relied approach for the coal HHV foretelling as stated in *GCV* criterion.

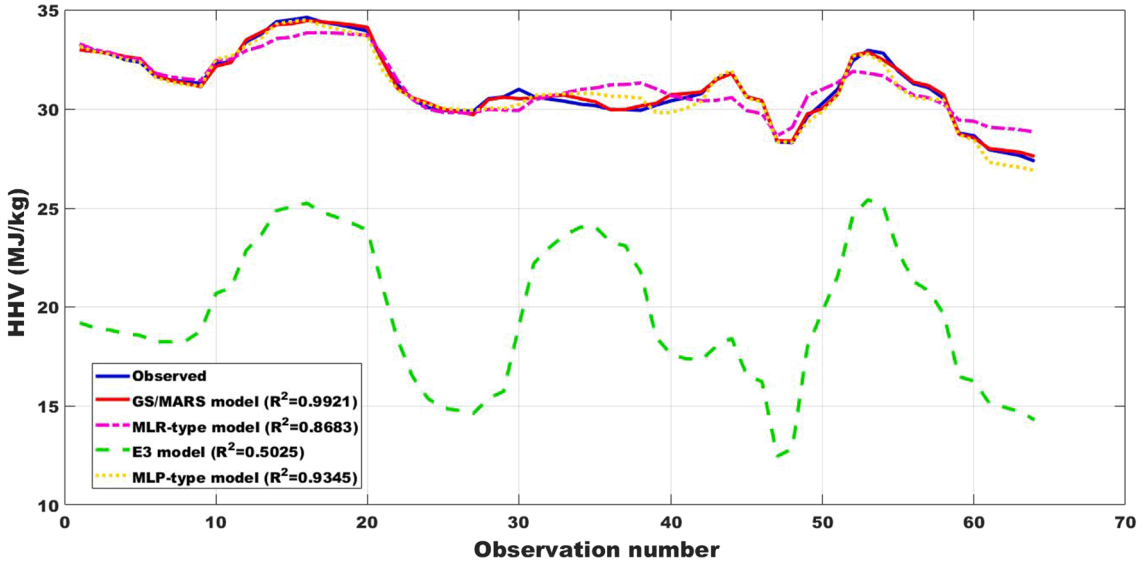

Fig. 8. Observed and predicted values of the coal HHV for the test set using: Channiwala and Parikh (E3) empirical correlation; MLR-type model; MLP-type model; and GS/MARS model.

both, i.e. (N) and (S), could be inferred in indirect mode by defect as part of the total composition of coal in the numerical approach. In this sense, the potential existence of theoretical models for HHV of solid fuels with strong relationships to (C), which show an effect with (H) and (O), among other ultimate composition elements, were highlighted by Boumanchar et al. (2019) [55]. The characterization of the solid fuel in relation with the heating value allows the implementation for thermal and power applications of energy systems [56,57].

In conclusion, this research successfully enables the estimation of the coal HHV output factor using the GS/MARS–relied approximation in agreement with the real observed values. Indisputable, Fig. 8 illustrates the comparison of experimental and foretold coal HHV values using the best empirical correlation (Channiwala and Parikh (E3) empirical correlation), MLR approach, MLP-type artificial neural network and GS/MARS-relied approximation. Therefore, with the purpose of achieving the best approximation for this regression problem, it is essential to use a MARS approach. These results unequivocally support the crucial statistical standard of 'goodness of fit' (R^2), demonstrating that the GS/MARS–relied approximation provides the best fit.

4. Conclusions

The key conclusions of this study can be summed up by comparing the numerical and experimental results as follows:

- Firstly, in order to determine the coal HHV factor, it is necessary to solve a difficult heat transfer problem that takes into account the three different types of heat transmission: conduction, convection, and radiation. The resolution of partial differential equations (EDPs) is implied by the ensuing complete model. In reality, numerical techniques are needed to solve these EDPs (such as the finite element method, the finite differences method, etc.), and some additional heuristic approximations result in solutions that are very different from one another. As a result, the discovery of new MLT–based analysis techniques is highly significant. In particular, the GS/MARS–relied approximation used in this study is a suitable option to evaluate the HHV variable in various types of coal with enough precision. Indeed, it was confirmed that the coal HHV can be exactly calculated in the fuel industry using a GS/MARS–relied approximation using testing data (20% experimental data not used for training), since a coefficient of determination with a value of 0.9921 is obtained.
- Secondly, due to the fact that MARS approximations produce an explicit mathematical expression of the coal HHV from the input variables as a summation of basis functions (hinge functions and the product of two or more functions of this kind), the MARS approach can be configured into a low-cost microcontroller-based device to achieve a reliable forecasting performance of coal HHV (fuel automation applications).
- Thirdly, it is possible to arrange the input variables used in the foretelling of the coal HHV in order of their significance. One of the main findings of this investigation is this. In this way, the Carbon content (C) could be considered the most significant predictor of the coal HHV output variable, followed by the contents of O, H, S and N, each in order.
- Finally, in future research, for the definition of hybrid models based on both proximate and/or ultimate analyses, the ideas presented here are very general and could, in theory, be broadened to include more independent variables.

To sum up, this GS/MARS approach could be successfully applied to other types of coals with similar or distinct origins, but it is essential to always consider the distinctive qualities of each deposit and basin.

CRediT authorship contribution statement

Paulino José García–Nieto: Writing – original draft, Software, Validation, Data curation, Conceptualization, Methodology, Validation, Formal analysis, Visualization, Investigation, Supervision, Writing – review & editing. **Esperanza García–Gonzalo:** Writing – review & editing, Writing – original draft, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **José Pablo Paredes–Sánchez:** Writing – original draft, Software, Validation, Data curation, Conceptualization, Methodology, Validation, Formal analysis, Visualization, Investigation, Supervision, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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