Mathematical model for predicting the formation of ferrous deposits during coal combustion

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Abstract. For the first time, on the basis of a combined model of the principal component method and neural network modeling method, a unified method for evaluating coals for the formation of strong ferrous deposits is proposed, taking into account the ash composition, combustion conditions and the degree of grinding. The results of predicting the propensity to form ferrous deposits of \( R_{fe} \) have shown acceptable accuracy of determination. Expanding the experimental database on different types of coals will improve the accuracy of modeling and the widespread use of this technique in the energy sector.

1. Introduction
One of the problems when burning coal dust in the furnace chamber is the formation of ferrous deposits. Strong ferrous deposits are formed from the products of incomplete oxidation of pyrite, ash and low-melting eutectic based on them. The formation of strong ferruginous deposits can be observed along the entire height of the furnace. These deposits form the primary layer of deposits and serve as the basis for the growth of slag deposits.

A significant number of papers were devoted to the study of iron-rich deposits [1-3]. The main factors that affect the intensity of bottom sediment formation were identified and methods for evaluating coals for the formation of strong ferruginous deposits were proposed based on experimental data. One of the most developed methods is the UralVTI method [1]. It considers the degree of coal metamorphism by dividing the coals into 5 groups and adopting different empirical coefficients for different groups. The influence of iron content and ash composition is taken into consideration. Despite the universality of the method, its application to "mechanically activated" coals does not take into account one of the main factors of "mechanical activation" in terms of sediment formation. This factor is associated with a decrease in the degree of grinding of coal.

The purpose of this work is to develop a unified methodology for evaluating coals for the formation of strong ferrous deposits, taking into account the ash composition, combustion conditions and the degree of grinding. A single functional dependence of the propensity to form ferrous deposits is described using neural networks without the conclusion of empirical dependences.

2. Problem statement and research methods
When constructing a method for calculating the intensity of ferruginous deposits, a normalized value of \( R_{fe} \) is introduced to quantify the propensity to form them. This value is determined by processing experimental data on coal and their combustion conditions, as well as by the results of inspection of boilers. Coals with a very high propensity to form ferrous deposits correspond to the normalized value of \( R_{fe} = 0.8 \) and those with a low propensity - to \( R_{fe} = 0.2 \) [4].
Data on 25 coals were used to develop the methodology. Tables 1, 2 and 3 present data for two coals out of 25. In the developed methodology, it was assumed that the normalized value of \( R_{fe} \) depends on the technical characteristics of the fuel (table 1), the ash composition (table 2) and the conditions of coal combustion (table 3). Experimental data presented in figure 1 [4] were used to account for the effect of fine grinding of coal on the formation of ferrous deposits. This figure shows the tendency to form ferrous deposits taking into account the degree of grinding based on the generalization of experimental data depending on the content of sulfur in coal.

### Table 1. Technical characteristics of the initial coals.

|          | \( W_{a} \) | \( A_{d} \) | \( V_{daf} \) | \( C_{daf} \) | \( H_{daf} \) | \( S_{daf} \) | \( O_{daf} \) | \( Q_{s,daf} \) |
|----------|--------------|-------------|--------------|---------------|---------------|---------------|---------------|----------------|
| Kuznetsk coal | 5.4          | 22.3        | 34.7         | 75.57         | 5.66          | 0.55          | 16.44         | 29.7           |
| Brown coal  | 30           | 12          | 46           | 71.4          | 4.0           | 0.3           | 13.7          | 26.1           |

### Table 2. Technical characteristics of the ash.

|          | SiO2 | Al2O3 | TiO2 | Fe2O3 | CaO | MgO | K2O | Na2O |
|----------|------|-------|------|-------|-----|-----|-----|------|
| Kuznetsk coal | 58.8 | 24.4  | 0.9  | 6.7   | 4.2 | 1.9 | 1.9 | 1.1  |
| Brown coal  | 53.5 | 12.3  | 0.6  | 7.2   | 21.4| 4.1 | 0.5 | 0.4  |

### Table 3. The conditions of coal combustion

|          | \( T^\circ \), \( °C \) | \( R_{fe} \) (standard grinding) | \( R_{fe}^* \) |
|----------|--------------------------|---------------------------------|----------------|
| Kuznetsk coal | 2004                     | 0.2                             | \( R_{fe}=f(R_{ot}, S_p^p) \) |
| Brown coal  | 1454                     | 0.6                             | \( R_{fe}=f(R_{ot}, S_p^p) \) |
A neural network modeling is one of the appropriate methods for establishing a single functional relationship between parameters based on available data. The neural network modeling method is used when the exact type of relationship between input parameters and output values is unknown. The layers are connected so that the signal from the inputs propagates through the network and reaches the outputs. The behavior of neural networks is determined in accordance with the functions of converting neurons, network topology, and the type of layer connection. Among all forms of neural networks, the most popular is the direct propagation network (multi-layer perceptron). This type of network consists of several layers of neurons. The neurons of the first layer (input) do not process any input information, but only distribute the signals sent to the network input between the neurons of the following layer. Their activation function is linear. Output layer neurons can be either linear or nonlinear. In fact, the network communicates with the ambient medium only through the neurons of these two extreme layers.

The main processing of information is performed by neurons of hidden layers with nonlinear activation functions that do not have connections to the ambient medium of the network. Inside the layers, connections between neurons are not allowed, and the flow of information goes only in one direction. Various types of sigmoid functions are usually selected as activation functions for hidden layer neurons. The network tuning parameters are weight coefficients, which are multiplied by the signals received at the neuron inputs from the neurons of the previous layer (Fig. 2).
Input parameters for the model are information about the chemical composition of ash, pyrite sulfur content, adiabatic combustion temperature, and fineness of coal grinding. Data deviation from standard grinding and change in the \( R_{fe} \) value was taken into account by the \( R_{fe} = f(R_{so}, S^d_p) \). For each of the coals, three different grinds with their own \( R_{fe} \) values were considered. The number of data sets is 75.

In this statement, the problem is an approximation of a continuous function using a multilayer perceptron. According to the universal approximation theorem [5, 6], a multilayer perceptron with one hidden layer is sufficient to construct an approximation for any training set represented by a set of input data \( x_1, x_2, \ldots, x_n \) and their responses \( f(x_1, x_2, \ldots, x_n) \).

This approximating function is represented as follows:

\[
F(x_1, \ldots, x_{1m_0}) = \sum_{i=1}^{m_1} \alpha_i \varphi(\sum_{j=1}^{m_0} \omega_{ij} x_j + b_i),
\]

where \( x_1 \) and \( x_{m_0} \) are the input parameters (attributes), \( m_1 \) is the number of neurons of the hidden layer, \( \alpha_i, \omega_{ij} \) are the weights of the layers of the neural network, \( b_i \) is the shift vector, \( \varphi \) is the activation function of the hidden layer, and \( F(x_1, \ldots, x_{m_0}) \) is the neural network model that approximates the target variable.

Rather limited data values for training leads to the need to reduce the amount of input data. One way to reduce the dimension of the input data space is to use the principal component method (PCA). The source data space is transformed in such a way that only "effective" features remain (that is a significant part of the information contained in the data). In addition, the principal component method allows you to speed up the learning process by back propagation by ensuring that there is no significant correlation of incoming values.

The training data consist of 15 parameters: a technical fuel composition, chemical composition of fly ash, the adiabatic temperature of combustion and the degree of the fuel grinding. The number of data sets is 75. The target parameter (that we want to learn to model) is the tendency to form ferrous deposits \( R_{fe} \).

The average relative error (MAPE) was used as a function of the model error, which was minimized during neural network training. We used the average relative error as a quality metric

\[
MAPE = \frac{100}{N} \sum_{i=1}^{N} \frac{|y_i - a_i|}{y_i},
\]

as well as the coefficient of determination

\[
R^2 = 100\% \left(1 - \frac{\sum_{i=1}^{N}(y_i - a_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2}\right),
\]

where \( a_i \) is the forecast of the model, \( y_i \) is the actual result, \( \bar{y} \) is the sample average, and \( N \) is the sample size.

The full sample of experimental data was divided into training and test samples in a ratio of 80% to 20%. The total number of training examples was 75. The quality of the model with optimal parameters was evaluated in a test sample. The main variable parameters in the model were: the number of main components from 3 to 8, and the number of neurons in the inner layer from 6 to 10. The tanh activation function was used for neurons in hidden layers, and the linear activation function was used for the output layer.

### 3. Results and discussion

Figures 3-6 show the results of calculations. It can be seen that if there are 4 main components (Fig. 3,4), the model results on the trained sample are acceptable (\( R^2=0.931 \)), but in the test sample, the model shows a significant error for both 6 and 10 neurons of the inner layer (table 4). The accuracy of calculations for the test sample increases when the number of main components is equal to 8 (Fig. 5,6).
Further increases do not reduce the calculation error. At the same time, increasing the hidden layer neurons from 6 to 10 also increases the accuracy of the calculation on the test sample.

From the model application to a test sample with the number of main components equal to 8 and 10 neurons of the inner layer, it is clear that the proposed approach gives an error in predicting the propensity of coal to form ferrous deposits of no more than 13%. Given the small training sample, this result can be considered acceptable. As experimental data is accumulated and added to the training sample, the accuracy of the estimate will increase.

![Figure 3](image3.png)

**Figure 3.** Results of modeling the $R_{fe}$ value. Blue dots are the training sample. Red dots are the test sample. PC=4, the number of neurons in hidden layer =6

![Figure 4](image4.png)

**Figure 4.** Results of modeling the $R_{fe}$ value. Blue dots are the training sample. Red dots are the test sample. PC=4, the number of neurons in hidden layer =10

![Figure 5](image5.png)

**Figure 5.** Results of modeling the $R_{fe}$ value. Blue dots are the training sample. Red dots are the test sample. PC=8, the number of neurons in hidden layer =6

![Figure 6](image6.png)

**Figure 6.** Results of modeling the $R_{fe}$ value. Blue dots are the training sample. Red dots are the test sample. PC=8, the number of neurons in hidden layer =10

| Table 4. Error modeling the $R_{fe}$ value |
|-------------------------------------------|
|                                          |
| PC=4, Neurons =6 | PC=4, Neurons =10 | PC=8, Neurons =6 | PC=8, Neurons =10 |
| Model training error (training sample)MAPE(%)$/R^2$ | 17.17 | 11.63 | 10.05 | 4.78 |
| The generalization error of the model (test sample)MAPE(%)$/R^2$ | 0.870 | 0.931 | 0.949 | 0.987 |
|                                          | 33.26 | 27.08 | 18.57 | 13.01 |
|                                          | 0.401 | 0.529 | 0.784 | 0.870 |
Conclusions
For the first time, a unified method has been proposed for evaluating coals for the formation of strong ferrous deposits, taking into account the ash composition, combustion conditions and the degree of grinding, based on a combined model of the principal component method and a neural network modeling method. The results of calculations on the test sample show that the proposed approach gives an error in predicting the propensity of coal to form ferrous deposits $R_{fe}$ of no more than 13%. To improve the accuracy of forecasting, it is necessary to expand the experimental database on different types of coals. In accordance with the results of calculations, this method can be used to determine the intensity of ferrous deposits when burning mechano-activated coals.

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