Conference Paper

Simulation of Coke Quality Indicators Using Artificial Neural Network

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Abstract

The article shows the application of a neural network for modeling coke quality indicators Coke Reactivity Index (CRI) and Coke Strength after Reaction (CSR). Two optimization methods were used to train the neural network. The influence of the number of neurons on the simulation results was studied. The difference between experimental and calculated data on average does not exceed 2 %. The conclusion is made about the prospects of using a neural network to predict the values of CRI and CSR of coke.

Keywords: artificial neural network, coke, coke reactivity index, coke strength after reaction

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1. Introduction

An important task of metallurgical coke production is to obtain coke of a given quality. It is known (see, for example, [1]) that metallurgical coke can be characterized by two parameters: CRI and CSR. At present, there is no reliable model for calculating CRI and CSR based on the characteristics of charge materials and coking mode. In this regard, studies in the direction of establishing the dependence of coke quality on the characteristics of the charge are relevant.

In studies in this direction, regression and correlation analysis methods are often used (see, for example, [2]). In [2], a linear regression dependence between CRI and CSR was obtained with a correlation coefficient of 0.97; the determination coefficients between CRI and the volume fraction of internite, vitrinite reflection index, hygroscopic humidity are in the range 0.26 – 0.27, which indicates a complex mutual influence of the factors considered.

It can be concluded that the problem of determining the characteristics of the quality of coke CRI and CSR can be attributed to an insufficiently formalized problem in which there are many influencing factors (for example, petrographic composition, degree of metamorphism, etc.), which are not always strictly possible to take into account.

Table 1: Charge composition and results of CRI and CSR determination

Component	Share, % (below the number of months)									
	1	2	3	4	5	6	7	8	9	10
Component 1	3	7,2	8,9	10,2	10,4	15,8	17,4	8,6	7,3	2,2
Component 2	43,4	39,4	38,0	38,9	35,1	26,4	30,7	36,9	36,8	42,0
Component 3	5,8	5,3	0,7	7,7	17,1	7,5	5,6	5,6	1,2	10,5
Component 4	9,9	5,8	16,0	9,0	10,5	20,5	8,5	11,0	12,1	6,8
Component 5	0,0	4,6	0,0	0,0	0,0	0,0	4,3	3,5	5,8	2,6
Component 6	19,1	24,2	13,0	9,1	5,0	3,4	1,3	8,8	6,1	11,7
Component 7	0,0	0,0	3,5	10,5	8,6	6,1	10,9	7,1	8,4	3,7
Component 8	8,8	7,9	6,5	2,3	2,9	6,4	14,0	14,5	18,3	16,5
Component 9	6,1	1,6	9,4	8,5	6,4	9,9	3,3	0,0	0,0	0,0
Component 10	3,9	4,0	4,0	3,8	4,0	4,0	4,0	4,0	4,0	4,0
CRI, %	56,2	56,2	55,6	54,6	55,9	56,1	54,9	56,0	56,1	55,1
CSR, %	30,2	30,2	30,3	30,6	30,2	30,5	30,5	30,2	30,2	30,4

The solution of insufficiently formalized problems is possible using artificial neural networks (see, for example, [3]). This approach was used in [2] to describe the quality of coke and in [4] to analyze the yield of chemical coking products.

To determine the weight matrices of a neural network, training examples are needed – the charge parameters and the values of CRI and CSR obtained for them. The data for the study and the results of the determination of CRI and CSR are provided by industrial enterprise and are shown in tables 1, 2.

2. Results and Discussions

A two-layer artificial neural network (TLANN) was used to simulate CRI and CSR, the structure of which is shown in Fig.1. The logistic function was used as a compressive function A two-layer artificial neural network (TLANN) was used to simulate CRI and CSR, the structure of which is shown in Fig. 1. The logistic function was used as a compressive function $F(x) = \frac{1}{1+e^{-x}}$ [5].

The number of neurons in the outer layer was chosen to be equal to two in the number of coke quality parameters CRI and CSR. The quantity in the inner (hidden) layer varied over a wide range to determine the effect of this factor on the simulation results.

Table 2: Characteristics of the charge

Component	Quality indicator,%									
	Ad	Vdaf	y	Sd	Vt	Sv	I	Ro,r	ΣOK	Io
Component 1	7,5	38,3	18,4	0,46	88	2	10	0,811	11,8	0,222
Component 2	8,0	36,7	28,2	0,56	86	2	12	0,935	13,0	0,265
Component 3	9,4	24,8	14,6	0,32	48	10	42	1,177	48,7	0,286
Component 4	7,8	20,9	11,3	0,29	57	11	32	1,383	39,1	0,327
Component 5	8,4	18,6	7,3	0,36	53	9	38	1,506	44,0	0,205
Component 6	9,3	18,5	8,9	0,34	51	10	39	1,464	45,8	0,241
Component 7	11,2	18,8	11,3	0,23	67	5	28	1,539	31,0	0,159
Component 8	7,9	20,1	10,8	0,37	50	11	38	1,357	45,7	0,251
Component 9	11,5	27,5	9,3	0,58	56	5	39	1,050	42,1	0,100
Component 10	0,3	19,1	0	4,70	99	0	1	2,340	0,5	0,878

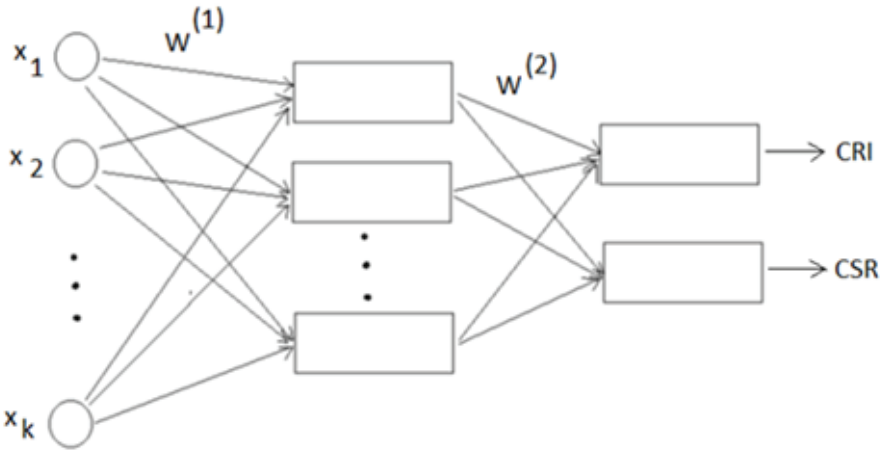

Figure 1: TLANN structure

10 training examples (according to the number of months from table 1), in each of which there were 10 parameters from the table.2 taking into account the content of the charge components.

To improve the quality of the simulation, the original data and results were preprocessed so that they were in a single range, usually from 0 to 1.

The method of error back propagation (see, for example, [5]) was used to train DEANS, in which the functional of the form was minimized

$$E(w) = \frac{1}{2}\sum_{t=1}^{T}\sum_{l=1}^{n}\left(y_{lt} - d_{lt}\right)^2 \to \min$$

Here T - the number of training examples to which the given result corresponds d_{lt} (these are the CRI and CSR values from the table 1); n – number of neurons in the output

layer (n=2); y_{lt}- the output of the neural network during its training (after training should be close to the values of CRI and CSR from the table.1).

The weight matrices were the minimization parameters w(1) and w(2) (see fig.1). The search for elements of the neural network weight matrices was carried out using two methods of unconditional optimization: the method of the steepest descent and the method of conjugate gradients (see, for example, [6]). In both approaches, it is necessary to determine partial derivatives of the functional E(w) on the elements of the weight matrices $w_{ij}^{(1)}$ and $w_{ij}^{(2)}$. The following expressions for partial derivatives were obtained

$$\frac{\partial E}{\partial w_{jk}^{(2)}} = \sum_{t=1}^{T} \left(y_{kt}^{(2)} - d_{kt} \right) \cdot (1 - F(S_{kt}^{(2)})) \cdot F(S_{kt}^{(2)}) \cdot y_{jt}^{(1)}, \quad j = 1...n, \quad k = 1...p. \tag{1}$$

$$\begin{aligned} \frac{\partial E}{\partial w_{ij}^{(1)}} &= \sum_{t=1}^{T} \sum_{l=1}^{p} \left(y_{lt}^{(2)} - d_{lt} \right) \cdot \left(1 - F\left(S_{lt}^{(2)} \right) \right) \cdot F\left(S_{lt}^{(2)} \right) \\ &\quad \cdot \left(1 - F\left(S_{jt}^{(1)} \right) \right) \cdot F\left(S_{jt}^{(1)} \right) \cdot x_{it} \cdot w_{jl}^{(2)}. \\ i &= 1...m, \quad j = 1...n. \end{aligned} \tag{2}$$

Formulas (1)-(2) determine partial derivatives of the target function E (w) by the weights of neurons of the second (external) and first (hidden) layers.

The symbols used here are

$$S_{jt}^{(1)} = \sum_{i=1}^{m} x_{it} \cdot w_{ij}^{(1)} \quad j = 1..n; y_{jt}^{(1)} = F(S_{jt}^{(1)}) = F\left(\sum_{i=1}^{m} x_{it} \cdot w_{ij}^{(1)} \right).$$

$$S_{lt}^{(2)} = \sum_{j=1}^{n} y_{jt}^{(1)} \cdot w_{jl}^{(2)} \quad l = 1..p; y_{lt}^{(2)} = F(S_{lt}^{(2)}) = F\left(\sum_{j=1}^{n} y_{jt}^{(1)} \cdot w_{jl}^{(2)} \right).$$

Corrections for weights, for example, in the method of the quickest descent at the step with the number are determined by the relations [6] (η- parameter of the method)

$$\Delta w_{ij}^{(1)\tau} = -\eta \cdot \frac{\partial E}{\partial w_{jk}^{(1)}}; w_{ij}^{(1)\tau+1} = w_{ij}^{(1)\tau} + \Delta w_{ij}^{(1)\tau}; \Delta w_{jk}^{(2)\tau} = -\eta \cdot \frac{\partial E}{\partial w_{jk}^{(2)}}; w_{jk}^{(2)\tau+1} = w_{jk}^{(2)\tau} + \Delta w_{jk}^{(2)\tau}.$$

Calculations Δw_{ij}^{τ} are terminated if Δw_{ij}^{τ} become less than the specified accuracy of calculations.

The result of TLANN application is expressed by matrix transformations

$$\begin{pmatrix} x_1 & \dots & x_m \end{pmatrix} \cdot \begin{pmatrix} w_{11}^{(1)} & \dots & w_{1n}^{(1)} \\ \vdots & \ddots & \vdots \\ w_{m1}^{(1)} & \dots & w_{mn}^{(1)} \end{pmatrix} = \begin{pmatrix} S_1^{(1)} \\ \vdots \\ S_n^{(1)} \end{pmatrix} \rightarrow \begin{pmatrix} F\left(S_1^{(1)} \right) \\ \vdots \\ F\left(S_n^{(1)} \right) \end{pmatrix} = \begin{pmatrix} y_1^{(1)} \\ \vdots \\ y_n^{(1)} \end{pmatrix}$$

and

$$\left(y_1^{(1)} \ \dots \ y_n^{(1)} \right) \cdot \begin{pmatrix} w_{11}^{(2)} & \dots & w_{1p}^{(2)} \\ \vdots & \ddots & \vdots \\ w_{n1}^{(2)} & \dots & w_{np}^{(2)} \end{pmatrix} = \begin{pmatrix} S_1^{(2)} \\ \vdots \\ S_p^{(2)} \end{pmatrix} \rightarrow \begin{pmatrix} F\left(S_1^{(2)}\right) \\ \vdots \\ F\left(S_p^{(2)}\right) \end{pmatrix} = \begin{pmatrix} y_1^{(2)} \\ \vdots \\ y_p^{(2)} \end{pmatrix}.$$

Table 3: The results of calculations in the framework of the fastest descent method

№ of month	Exper-ience	Exper-ience	7 neurons in the 1st layer				10 neurons in the 1st layer			
			model		error, %		расчет		error, %	
	CRI, %	CSR, %	CRI, %	CSR, %	CRI, %	CSR, %	CRI, %	CSR, %	CRI, %	CSR, %
1	56,20	30,20	55,72	30,21	0,85	0,03	55,8	30,1	0,71	0,33
2	56,20	30,20	56,96	29,08	1,35	3,71	57,24	28,8	1,85	4,64
3	55,60	30,30	55,43	30,54	0,31	0,79	55,27	30,69	0,59	1,29
4	54,60	30,60	55,44	30,56	1,54	0,13	55,23	30,79	1,15	0,62
5	55,90	30,20	55,66	30,38	0,43	0,60	55,46	30,61	0,79	1,36
6	56,10	30,50	56,57	29,60	0,84	2,95	56,54	29,69	0,78	2,66
7	54,90	30,50	56,59	29,52	3,08	3,21	56,9	29,27	3,64	4,03
8	56,00	30,20	54,9	30,99	1,96	2,62	54,82	31,03	2,11	2,75
9	56,10	30,20	54,42	31,42	2,99	4,04	54,35	31,43	3,12	4,07
10	55,10	30,40	55,02	30,83	0,15	1,41	55,14	30,67	0,07	0,89
Average					1,35%	1,95%			1,48%	2,26

The results of calculations together with experimental data (table 1) for some optimization methods are given in tables 3, 4. From this data, it can be concluded that the conjugate gradient method gives the best average accuracy of the calculations for CRI and CSR. The maximum error when using the steepest descent method is 4.64%, and the conjugate gradient method is 2.66%. Increasing the number of neurons in the inner layer from 7 to 10 leads to an increase in the average error of calculations for CRI and CSR.

A visual representation of the consistency of calculation results CRI and CSR for the number of neurons in the inner layer equal to 7 shown in Fig. 2, 3. From these data, it can be concluded that the TLANN used allows a satisfactory description of the experimental data. for the number of neurons in the inner layer equal to 7 shown in Fig. 2, 3. From these data, it can be concluded that the TLANN used allows a satisfactory description of the experimental data. The calculations were performed using a own C# program.

Table 4: Results of calculations in the framework of the conjugate gradient method

№ of month	Experience	Experience	7 neurons in the 1st layer				10 neurons in the 1st layer			
			model		error, %					
	CRI, %	CSR, %	CRI, %	CSR, %	CRI, %	CSR, %	CRI, %	CSR, %	CRI, %	CSR, %
1	56,20	30,20	55,89	30,06	0,55	0,46	55,99	29,92	0,37	0,93
2	56,20	30,20	56,57	29,44	0,66	2,52	56,44	29,52	0,43	2,25
3	55,60	30,30	55,43	30,56	0,31	0,86	55,41	30,57	0,34	0,89
4	54,60	30,60	55,12	30,87	0,95	0,88	55,05	30,96	0,82	1,18
5	55,90	30,20	55,3	30,72	1,07	1,72	55,25	30,81	1,16	2,02
6	56,10	30,50	56,12	30,01	0,04	1,61	56,21	30,01	0,20	1,61
7	54,90	30,50	56,28	29,8	2,51	2,30	56,36	29,77	2,66	2,39
8	56,00	30,20	55,24	30,68	1,36	1,59	55,15	30,74	1,52	1,79
9	56,10	30,20	55,1	30,79	1,78	1,95	55,08	30,76	1,82	1,85
10	55,10	30,40	55,62	30,28	0,94	0,39	55,73	30,11	1,14	0,95
Average					1,02%	1,43%			1,05%	1,59%

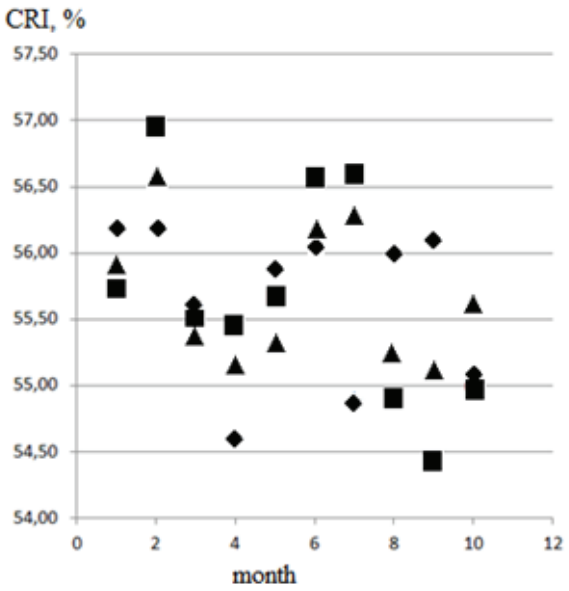

Figure 2: Comparison of experimental data and results of CRI calculations. Diamonds-experimental data; squares - results of calculations by the method of the fastest descent; triangles - results of calculations by the method of conjugate gradients

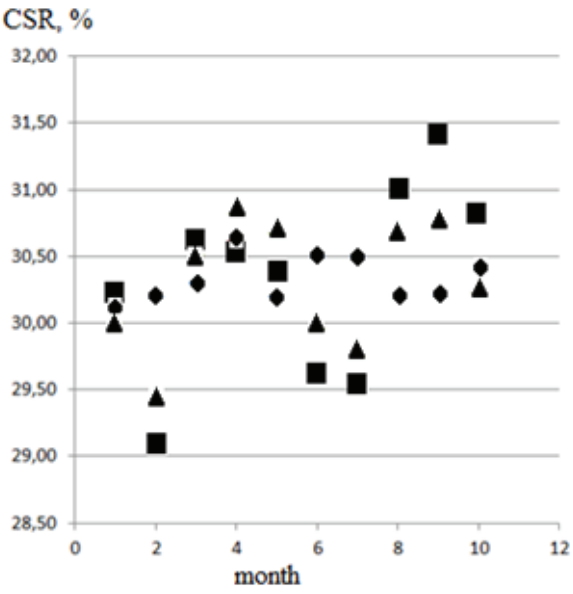

Figure 3: Comparison of experimental data and results of CSR calculations. Diamonds-experimental data; squares - results of calculations by the method of the fastest descent; triangles - results of calculations by the method of conjugate gradients

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