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Blast Furnace Slag Viscosity Prediction based on GRNN

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Abstract

Viscosity is the basic physical property of metallurgical blast furnace slag, which directly affects the reaction rate, slag separation effect and many other smelting properties. However, the measurement of slag viscosity at high temperature is costly and time-consuming, and the traditional viscosity prediction model is not satisfactory, and the operation is complicated, which is not conducive to researchers' experiments. Therefore, it is of great significance to develop multi-component viscosity prediction model algorithm. Based on the main components of blast furnace slag MgO-CaO-Al_2O_3-SiO_2 and temperature as influencing factors, the basic prediction model is constructed by using generalized neural network theory. By preprocessing and dividing the existing 1000 groups of data, the optimal value of sigma is obtained by grid search algorithm. The results show that the prediction accuracy of the algorithm reaches 87.2% when sigma=1.101. Compared with the accuracy of 80% of the traditional viscosity prediction model, it has a great improvement. The algorithm has high applicability, can meet the basic viscosity prediction, can solve the demand that the data of scientific researchers are difficult to obtain, and has certain popularization significance.

Keywords

Generalized Neural Network Theory; Grid Search Algorithm; Viscosity Prediction; Blast Furnace Slag.

1. Development Background and Significance

1.1 Present Situation of Blast Furnace Slag Treatment

China now advocates the implementation of the "green steel" policy. At present, iron and steel enterprises will produce 300~350 tons of blast furnace slag for every ton of pig iron. Blast furnace slag is the main waste produced after blast furnace ironmaking, which can be used as a silicate material with good performance. Its main components include CaO, MgO, Al_2O_3 and SiO_2. In the treatment of blast furnace slag, in addition to high energy consumption, gases such as steam, sulfur dioxide and hydrogen sulfide are also produced. After treatment, molten slag can be used as a good raw material for cement, and can be used instead of natural stone for pavement infrastructure, for preparing slag macadam concrete and for soft foundation. According to statistics, China's existing metallurgical enterprises spend as much as 100 million yuan on blast furnace slag waste every year. Therefore, the disposal and reuse of blast furnace slag is an effective way to promote the rapid development of circular economy in iron and steel industry, and it is also the key to realize green iron and steel.

1.1.1 Current Situation Abroad

Take the developed countries in the United States, Japan and the European Union as examples, the utilization fields of steel slag are mainly used for internal consumption of steel slag, cement, roads, buildings, civil engineering, etc., especially the use of steel slag in roads and internal circulation of steel mills; In the fields of cement and construction, the utilization rate of steel slag is still very low, but the overall utilization rate is generally high, with the utilization rate of steel slag in Japan as high

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as 98.4%. For example, Table 1[1-5] shows the utilization status of steel slag in the United States, Japan and European Union countries:

Table 1. Utilization Status of Steel Slag in USA, Japan and EU Countries

	Inner loop	Road	Cement	Build	Civil engineering	Temporary storage	Other	Undisposed
American	-	49.7	3.3	-	16	-	15.4	15.6
Japan	20.8	32.4	3.4	3.9	30.9	-	7	1.6
EU	11	43	5	3	3	19	3	13

The treatment methods of blast furnace slag abroad mainly include hot splashing method, slag crushing method, hot stewing method and flotation method. Japan uses steam aging method to treat steel slag, but because of its long cycle, it has developed a method of accelerated aging with steam in tanks, which greatly improves the efficiency of steel slag treatment [6]; In Germany, sand containing SO_2 and oxygen are added to molten steel slag to solidify f-CaO and f-MgO in steel slag, thus realizing steel slag treatment [7]. In Canada, Britain and India, hot splashing method is mainly used to treat steel slag [8]. These methods have certain advantages, but there are also some problems, such as there is still a certain amount of residual iron in the slag, and it needs to consume a lot of energy and chemicals.

1.1.2 Domestic Status Quo

At present, the blast furnace slag treatment methods used in production in China are basically water quenching treatment and dry treatment. Water quenching treatment is to put the molten blast furnace slag in water for cooling, so that its crystallization behavior is restricted. Then, under the action of thermal stress, the blast furnace slag will be granulated, and finally, after water quenching, sandy granulated slag will be obtained. However, this treatment method also has some problems, such as consuming a lot of water resources, producing a lot of sulfide, which will cause serious environmental pollution, and the recovery rate of residual heat of slag is low. At the same time, the water slag system also has some problems such as high energy consumption and heavy workload of system maintenance.

Because the research and application of the secondary resource recycling of blast furnace slag in China started late, only 30% of the steel slag has been effectively utilized at present, and the unused proportion is as high as 70%. There is still a big gap between China's steel slag treatment and developed countries, so China has a long way to go in steel slag treatment.

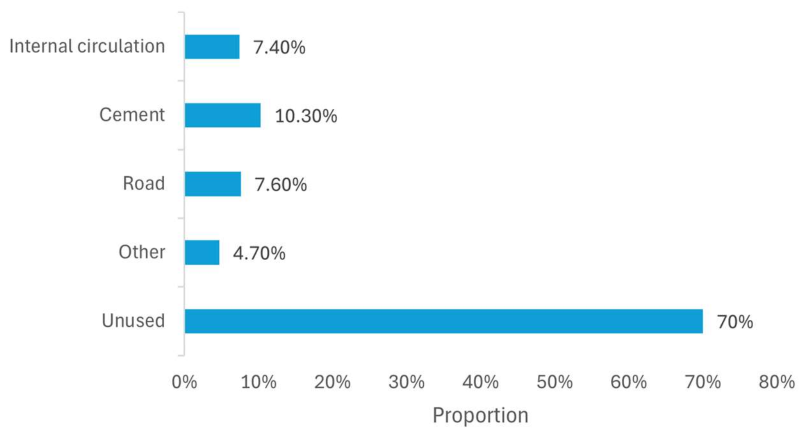

Figure 1. [10-12] Utilization Status of Steel Slag in China

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1.2 Present Situation of Slag Viscosity Prediction

Viscosity is the basic physical property of metallurgical slag, which directly affects the reaction rate, slag separation effect and many other important smelting processes. Moreover, when slag is widely used as the raw material of silicate materials, the viscosity of slag also plays a vital role in many other high-temperature industrial processes such as ceramics and glass manufacturing. Therefore, slag viscosity is an important index to guide production and new technology development.

With the gradual consumption of high-quality resources and the promotion of circular economy, as well as the increasing use of low-grade raw materials and solid wastes, the composition of iron smelting furnace materials will become more complex (high mass fraction of TiO_2, Cr_2O_3, etc.), resulting in complex slag composition and viscosity properties. However, viscosity measurement at high temperature is costly, time-consuming and laborious. Therefore, it is of great significance to develop viscosity calculation model and accurately simulate multi-component viscosity prediction model to improve the efficiency of metallurgical process.

In recent years, metallurgical workers have been deeply studying the viscosity of slag. The existing research results are mainly based on the influencing factors of slag viscosity, and the relationship between slag viscosity and chemical composition, structure and temperature is found on the basis of experimental data, so as to establish the testing method and prediction model of slag viscosity.

According to the modeling principle, the commonly used viscosity models are classified into four categories: viscosity-temperature dependence equation (such as Arrhenius model, Vogel-Fulcher-Tammann model, Adam-Gibbs model, Eyring model, etc.), component fitting model, structure model and solid-liquid coexistence multiphase viscosity model. These models have certain applicability and limitations. These models integrate structural information by physical or chemical methods, and establish the empirical relationship between viscosity and variables by mathematical methods.

Hou Liming et al.[9]studied the viscosity of CaO-SiO_2-Al_2O_3-FeO-MgO five-component slag system and the relationship between components and viscosity, and built an ANN-GA prediction model based on WEB neural network. The prediction of the viscosity of high FeO slag system shows that it is in good agreement with the experimental data, and the error is less than 20%.

Tang Xulong and others [13] deeply explored the relationship between slag viscosity and its structure, and on the basis of analyzing the relationship between slag viscosity and its (NBO/T) ratio (that is, the amount of non-bridging oxygen possessed by a single polymer particle), put forward a multi-component slag viscosity calculation model based on the (NBO/T) ratio. Firstly, the viscosity calculation model of $SiO_2 - \sum MxO$ simple slag system is established, and the model parameters are obtained by fitting the viscosity data of pure oxide and SiO_2–MxO binary slag system, and the average fitting error is between 9% and 18.5%. Subsequently, the model was extended to multi-component slag system. Based on the model parameters of SiO_2-MxO binary system, the model parameters of SiO_2–Al_2O_3–MxO ternary system were fitted, and the model parameters of slag system containing Al_2O_3 were obtained. The average fitting error was between 10% and 25%. The viscosity of SiO_2-Al_2O_3-CaO-MgO-FeO-Na_2O-K_2O-Li_2O-BaO-SrO-MnO composite slag system and its children was obtained by the established mathematical model, and the average error was less than 25%, and the prediction result was good. Based on the slag structure theory and referring to the empirical model, the model is superior to the traditional empirical model in prediction effect and application scope.

Chen Ziwei et al. [14] developed a structure-based artificial neural network (SIANN) model for the first time to predict the viscosity of slag. (i) A database containing 1892 reliable samples was established, and the quantitative atomic information of each sample was calculated by using the improved quasi-chemical model; (ii) using feedforward four-layer neural network to find and deal with the complex and subtle relationship between viscosity and influencing factors; (iii) The contribution of composition, temperature and structural characteristics to the model is evaluated by Olden and Jackson's connection weight method for the first time. The results show that after the quantitative atomic information is integrated into the model, the ability of the model to accurately

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predict viscosity is significantly improved, and the minimum prediction deviation is realized in various component systems.

The existing slag viscosity models can be divided into theoretical model, empirical model and semi-theoretical semi-empirical model from the construction principle. Based on the material structure, the theoretical model deduces the analytical expression of melt viscosity according to the principles of quantum mechanics and statistical thermodynamics. This kind of model has clear physical meaning, but its application scope is narrow and its extensiveness is small. The empirical model is the expression of viscosity obtained by direct fitting of experimental data. The physical meaning of this model is not clear, but the calculation results are more accurate in a certain range. Based on the theoretical model, the semi-theoretical semi-empirical model is modified by combining the experimental data, which makes the calculation result more accurate and the application scope more extensive.

However, these models need to be fitted by experimental data, and contain more empirical parameters, so their application scope is limited, and it is still impossible to predict the viscosity of blast furnace slag conveniently and quickly [15].

1.3 Significance of Viscosity Prediction

(1) In view of the problem that high alumina iron ore causes high W(Al_2O_3) in blast furnace slag at present, the viscosity prediction of blast furnace slag can adjust the metallurgical properties of slag according to the demand;

(2) The viscosity of slag affects the air permeability of the column below the slag-forming zone. Too high viscosity of slag will lead to unsmooth flow, reduce the porosity of coke skeleton, increase gas resistance and affect the smooth operation of blast furnace. Viscosity prediction is helpful for the smooth operation of blast furnace, and predicting the viscosity of slag system in the furnace quickly in advance can prevent the blockage of blast furnace and make timely measures to reduce the viscosity of blast furnace slag.

(3) The viscosity of slag affects the desulfurization ability of slag. Slag with low viscosity and good fluidity is beneficial to desulfurization, while slag with high viscosity and poor fluidity is not conducive to desulfurization. This is because the slag with low viscosity is beneficial to the diffusion of sulfur ions and promotes the desulfurization reaction. Viscosity prediction can predict the desulfurization ability of slag, judge whether it meets the standard of desulfurization reactant, and make adjustment measures in time;

(4) Slag viscosity affects slag tapping operation, and slag with too high viscosity is stuck in the ditch, which makes slag tapping difficult.

(5) The viscosity of slag affects the service life of blast furnace. The slag with high viscosity is easy to form slag skin in the furnace, which plays a role in protecting the lining, while the slag with too low viscosity and too good fluidity washes the lining and shortens the service life of blast furnace. Viscosity prediction can make timely measures to adjust the viscosity of blast furnace slag, protect the functional operation of blast furnace and prolong its service life.

(6) Direct measurement is a traditional way to obtain the viscosity of slag, but it is time-consuming and laborious to measure the viscosity at high temperature and has no practical significance. Therefore, the viscosity calculation model becomes an effective means to obtain the viscosity of slag.

1.4 Research Objectives

Based on the generalized neural network theory (GRNN), the viscosity values of blast furnace slag with different mass fractions of CaO, MgO, Al_2O_3 and SiO_2 at different temperatures are studied. Taking these main influencing factors as the input of the model and the final viscosity as the output of the model, a GRNN-based viscosity prediction model is established, and finally a software with viscosity prediction function is designed according to this model.

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In addition, when measuring viscosity, considering the influence of solid phase in the melt, different shear rates and crystallization behavior of slag will have an impact on the finally measured viscosity coefficient. Therefore, the following software design will consider these two factors and use them as the input of the model, and then promote and use them.

2. Introduction to the Principle of Developing Viscosity Prediction Software

2.1 Introduction of GRNN Algorithm

GRNN is a new type of RBF neural network, which has strong nonlinear mapping ability and fast learning speed. In the case of a large number of samples, it finally converges to the optimal regression, and it can still maintain good prediction performance in the case of a small number of samples, and can also effectively deal with unstable data. Although the accuracy of GRNN is not as good as that of RBF neural network, it has obvious advantages in classification and fitting, especially in the case of low data accuracy.

(1) Data preprocessing

First, check and clean the data, and keep 2 valid data.

Secondly, in order to avoid the influence of index dimension, the data is normalized by maximum-minimum method:

$$x_{inew} = \frac{x_i - x_{imin}}{x_{imax} - x_{imin}} \tag{1}$$

Where x_{inew} is the normalized data in column I, x_i is the original data in column I, x_{imax} is the maximum value in column I, and x_{imin} is the minimum value in column I.

Then the dependent variable (steel slag viscosity y) is converted into a column vector:

$$\mathrm{y} = \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \quad \mathrm{n} \in [1, +\infty) \tag{2}$$

* Description: Because Y will change with different X contents, there are five X quantities, and the changes of X quantities are close to countless, so the range of N is +∞.

(2) Model construction

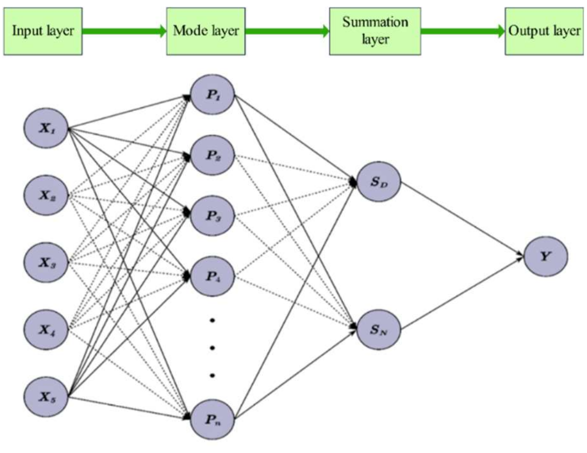

Fig. 2 Algorithm Structure Diagram

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According to the literature and related data, it is determined that there are five main factors that affect the viscosity of blast furnace slag, namely MgO, CaO, Al_2O_3, SiO_2 and T (temperature). Therefore, these five factors are selected as five indicators of the viscosity prediction model, namely, independent variables X_1, X_2, X_3, X_4 and X_5, and the viscosity is taken as the dependent variable (Y) for prediction.

In the figure, GRNN is a four-layer network structure, which is realized by the following four steps:

1) Input layer

The number of neurons in this layer corresponds to the number of input variables, that is, five, and the input data is transmitted to the mode layer.

2) Mode layer

This layer generally uses Gaussian function to process the data in the input layer, and the number of neurons is equal to the number of training samples. The transfer function of each neuron is:

$$p_i = exp\left[-\frac{(X-X_i)^T(X-X_i)}{2\lambda^2}\right] \qquad i = 1,2,3\cdots n \tag{3}$$

Where X_i is the training sample and λ is the smoothing factor.

3) Summation layer

When the dimension of output sample is 1, the number of nodes in this layer is 2, in which the output S_D of one node is the arithmetic sum of the output of mode layer, and the output S_{Nj} of other nodes is the weighted sum of the output of mode layer. The specific calculation formula is as follows:

$$S_D = \sum_{i=1}^{n} P_i \tag{4}$$

$$S_{Nj} = \sum_{i=1}^{n} y_{ij} P_i$$

Where P_i is the transfer function of the i-th neuron in the mode layer; Y_{ij} is the connection weight of the I-th neuron in the mode layer and the J-th molecular summation neuron in the summation layer.

4) Output layer

There is only one neuron in this layer, namely viscosity. Divide S_{Nj} and S_D to get the output result. The calculation formula is as follows:

$$Y_i = \frac{S_{Nj}}{S_D} \tag{5}$$

(3) Model parameter tuning

The core idea of GRNN algorithm is to use kernel density estimation to fit data distribution. In kernel density estimation, when we choose Gaussian kernel function as kernel, kernel density estimation becomes Gaussian kernel density estimation. The advantage of Gaussian kernel function is that it is easy to implement and usually gives good results for different data sets.

Sigma value is an important parameter of Gaussian kernel function, which determines the width of Gaussian distribution, thus affecting the overall performance of the model. When the sigma is smaller,

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the Gaussian distribution will become sharper, so only a few training samples have an impact on the prediction of the model, which leads to the over-fitting of the model. When the sigma is larger, the Gaussian distribution will become flatter, so many training samples will have an impact on the model, resulting in the model under-fitting.

Therefore, it is very important to select a suitable sigma value for the prediction of the model. At present, the grid search method is often used to search for the optimal value. This method lists the possible parameter combinations and carries out cross-validation under each combination to determine the final parameter value. Scholars use the network search module in the python language sklearn library to solve the sigma value of the optimal solution. The results show that the model is better when sigma=1.101.

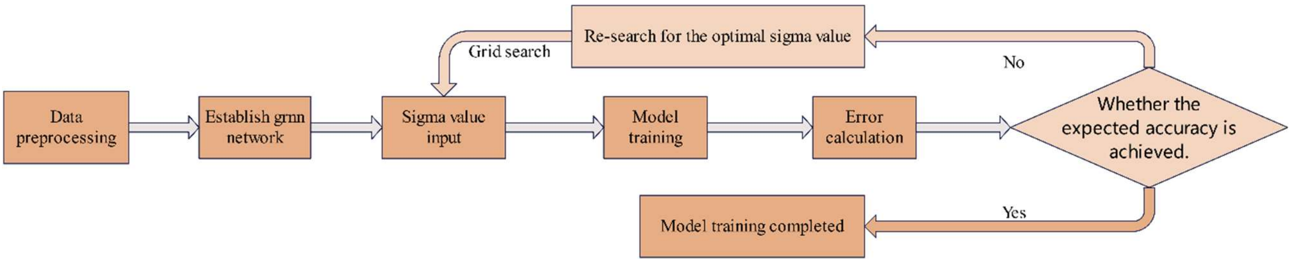

Fig. 3 algorithm flow chart

(4) Advantages of algorithm

When using traditional neural network to predict data, BP neural network has some shortcomings in the process of data prediction, such as slow convergence speed and local minimum, which leads to poor results in solving the problems of less sample size and more noise.

In contrast, GRNN has strong advantages in approximation ability, classification ability and learning speed. The network finally converges to the optimal regression surface with the largest sample size accumulation, and the effect is also good when the data is lacking. Moreover, the training of GRNN model does not need iteration, so it has fast training speed, good generalization ability, strong robustness, strong fault tolerance and flexible network structure. At the same time, GRNN has been widely used in signal process, structural analysis, education, energy, food, medicine, finance, biology and other fields.

2.2 Model Accuracy

According to consulting relevant data and literature, the ratio of most neural network training sets to test sets is 9: 1. Therefore, scholars divide the existing 1000 groups of data into training sets: test sets = 9: 1 to train and predict the model, and then calculate the error and accuracy of the algorithm, as shown in the following table:

Table 2. Algorithm Error and Accuracy

Proportion	RMSE	MAE	MSE	Accuracy rate
9:1	12.16	1.22	147.88	87.2%

Formula in the table:

$$\text{root}-\text{mean}-\text{square error}: RMSE=\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_j-y_i)^2}$$

$$\text{mean}-\text{squared error: } MSE = \frac{1}{n}\sum_{i=1}^{n}(y_j - y_i)^2$$

$$\text{Average absolute error: } MAE = \frac{1}{n}\sum_{i=1}^{n}\left|y_j - y_i\right|$$

Where n is the number of test sets, y_j is the predicted value and y_i is the true value.

As can be seen from the figure, when the ratio of training set to test set is 9: 1, the overall values of RMSE, MAE and MSE are smaller, especially the MAE value, which is a commonly used index to evaluate the accuracy of the model because it is insensitive to abnormal values and can well reflect the average error of model prediction. Therefore, the accuracy of the model is high at this time.

Therefore, when the selection ratio is 9: 1, the error of the model is only 12.8% (within the acceptable range), and the accuracy is as high as 87.2%. Compared with the 70% accuracy of the traditional prediction model, the accuracy of steel slag viscosity is greatly improved.

3. Feasibility Analysis

3.1 Data Source

The data from the experiment is authentic, but the obtained data will inevitably cause errors due to improper operation. The following is the part with data to show the content, actual data and forecast data of four components.

Table 3. Data Forecast Chart

MgO	CaO	Al_2O_3	SiO_2	Temperature	Actual	Predicted	Absolute difference
5.15	21.06	5.04	30.71	1450.00	9.39	8.94	0.45
1.51	22.78	6.63	29.08	1450.00	12.92	9.03	3.89
10.93	34.55	11.88	28.73	1450.00	3.46	4.26	0.80
6.01	33.41	15.89	37.96	1450.00	9.34	7.39	1.95
7.98	32.70	14.74	38.19	1450.00	8.05	7.28	0.77
2.54	27.12	14.29	33.74	1450.00	15.56	11.50	4.06
7.43	37.66	17.44	29.58	1450.00	4.89	5.16	0.27
9.08	48.87	11.53	37.18	1450.00	3.19	3.53	0.34
8.18	46.66	5.69	38.26	1450.00	2.70	3.48	0.78
8.67	48.87	19.72	25.71	1450.00	3.02	3.24	0.22

3.2 Feasibility Analysis of the Algorithm

The algorithm has been able to realize the basic viscosity prediction of blast furnace slag. In this algorithm, python language is used to predict the viscosity of blast furnace slag. The independent variables are divided into MgO, CaO, Al_2O_3, SiO_2 and temperature, and the dependent variables are viscosity values. When generalized neural network regression is used, the prediction accuracy reaches 87.2%, which is in line with the initial expectation.

3.3 The Scientific Advancement of the Algorithm

(1) Technological innovation: This work belongs to the innovative work of viscosity prediction, which is compiled and updated by Python language. Considering the influence of MgO-CaO-Al_2O_3-SiO_2 and temperature, a prediction model based on generalized neural network theory is established.

(2) Research value: Metallurgists are constantly studying the slag viscosity. Starting from the influencing factors of slag viscosity, based on the experimental data, the relationship between slag viscosity and chemical composition, structure and temperature is found, so as to establish the test method and prediction model of slag viscosity. Compared with the traditional viscosity prediction model, the viscosity prediction model established by this algorithm is simple to operate, which is beneficial for researchers to carry out experiments.

(3) Practical value: The accuracy rate of this model is 87.2%, which is improved to some extent compared with the existing viscosity prediction of multi-element complex slag system. It has high reference value and can be used by most scientific researchers. In the preliminary data preparation stage, the calculation data is used as a reference to facilitate the next experiment. In addition, the algorithm has high applicability, can meet the basic viscosity prediction, and has certain popularization significance.

4. Feasibility Analysis

The paper presents a viscosity prediction model for blast furnace slag based on the generalized regression neural network (GRNN) algorithm. The model utilizes MgO, CaO, Al_2O_3, SiO_2, and temperature as input variables and slag viscosity as the output variable. After preprocessing and dividing the data into training and testing sets, the optimal value of the sigma parameter is determined using grid search. The model demonstrates an accuracy rate of 87.2%, surpassing the traditional viscosity prediction model by 8.79%. This high accuracy is attributed to the GRNN algorithm's strong nonlinear mapping capability, fast learning speed, and good generalization ability. The proposed software is designed to be user-friendly and capable of meeting basic viscosity prediction needs. Additionally, the model has the potential for further improvement by considering the effects of solid phase content, shear rate, and crystallization behavior. In conclusion, the GRNN-based viscosity prediction model for blast furnace slag offers a simple and efficient solution for researchers and engineers in the field of metallurgy.

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