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Artificial Neural Network Prediction Model for Supercritical Water Gasification Data of Discarded Circuit Boards

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The gasification reaction is affected by the non-linear effects of temperature, pressure, feedstock concentration and other aspects due to the complexity of supercritical water. The conventional production forecasting methods have difficulties to predict conversion rates and yield of gas accurately. In this paper, an artificial neural network model is established to predict and analyse the conversion rates and the yields of gas products. The gasification experiment is carried out at different conditions. The data are taken as the learning samples, and 60 % of them are used for training and testing. Experimental data at different working conditions are randomly selected and inputted into the gasification artificial neural network model for prediction and analysis. The prediction accuracy of the carbon conversion rate of waste circuit boards is calculated whose coefficient of determination (R^2) is 0.98 and root mean square error (RMSE) is 2.22. In addition, R^2 of hydrogen yield is 0.85, and the deviation RMSE is 1.16. The prediction results of the neural network model constructed in this paper are in good agreement with the experimental data. And the model could realize the accurate prediction of the conversion rates of both carbon and hydrogen, and gas yield of discarded circuit boards. It is found that a double hidden layer neural network model is suitable for the prediction and analysis of the conversion rates while the single hidden layer neural network model suits for the prediction of hydrogen yield. Results at different reaction conditions can be obtained by this model and a lot of resources are saved in industrial design.

1. Introduction

Machine learning appeared in 1950s, which was used to imitate the way that humans learn by computer. Machine learning has gradually played a very important role in industrial applications. Zhu et al. (2020) established a machine learning model, and based on this model, the large-scale highly analytically simulated big data was used to predict the resistance of the filtered sub-grid, to correct the particle's resistance. Zhao et al. (2021) developed a machine learning (ML) framework to predict hydrogen production from supercritical water gasification of biomass. Their results showed that the R^2 of the prediction is 0.978. The research focused on the hydrogen yield, reaction efficiency and exergy efficiency. However, the yield of each gas composition and the conversion rates were not discussed. Shenbagaraj et al. (2021) developed multi-layered feed-forward back-propagation algorithm based artificial neural network (FFBPNN) models on food wastes' gasification, in which best prediction accuracy for CO yield prediction is achieved. The research focused on the gas compositions and yields instead of the conversion rates. Haq et al. (2022) used four different machine learning methods to find out the correlation between proximate, ultimate analysis and gasification conditions with H_2 production.
To report the results of gasification comprehensively, this paper focuses on the conversion rates and yield of gas. A model for accurately predicting the hydrocarbon gasification rate and gas yield is constructed. Based on a sufficient sample capacity, that is training and testing by plenty of experimental gasification data, the model could reach high accuracy for prediction. In this way, not only a lot of resources are saved, but also the obtained results provided for the design of reactors in industrial applications.

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2. Material and methods

2.1 Neuron model

The function of the neuron structure is to instantly perform calculation processing on the input vector data according to the set transition function and output the vector calculation result. The output vector structure of the neuron model will be affected by the input data vector, the activation function and the internal factors of the model. In order to eliminate the internal influence of the model, when the artificial neuron model is constructed, an additional input signal called deviation will be provided. The deviation value inputted is always 1.
The weights and input components can be represented by the following vector matrix Eq(1) and Eq(2) while the output vector of the neuron structure can be expressed as Eq(3).

$$W = \left[w_1, w_2, ..., w_r\right] \tag{1}$$

$$P = \left[p_1, p_2, ..., p_r\right]^T \tag{2}$$

$$A = f(W \cdot P + b) = f\left(\sum_{j=1}^{r} w_j p_j + b\right) \tag{3}$$

2.2 Backpropagation neural network model

The core algorithm in this paper is the backpropagation algorithm, a process of continuous training and optimisation of parameters. It consists of two steps, a forward-propagation calculation step for the information vector and a back-propagation update step for the error gradient. In algorithm's operation, the process of parameter solving is a process of continuous optimisation of the model. In each iteration, it will continue to advance in the direction of gradient decline and update the parameter value of each iteration.
The implementation steps are as follows:
1. Initial values of weights and bias items are set and random parameters will be automatically generated when calling Keras. The parameters are recorded as: $w^{(0)}, b_1^{(0)}, v^{(0)}, b_2^{(0)}$
2. The forward propagation calculation process of the input information vector is started with the input of the initial value, and the expected value of the output loss function of each layer is obtained:

$$E(\theta) = \frac{1}{2}\sum_{i=1}^{2}\left(y_i - \hat{y}_i\right)^2 \tag{4}$$

3.Error term of output vector of each layer of neural network is calculated according to the chain rule:

$$\nabla(k)v = \frac{\partial E}{\partial v} = \frac{\partial net_2}{\partial v}\frac{\partial \hat{y}}{\partial net_2}\frac{\partial E}{\partial \hat{y}} \tag{5}$$

4.The weights and bias terms of the output vectors of each layer of neural network are updated:

$$\nabla(k)w = \frac{\partial E}{\partial w} = \frac{\partial net_1}{\partial w}\frac{\partial h}{\partial net_1}\frac{\partial net_2}{\partial h}\frac{\partial \hat{y}}{\partial net_2}\frac{\partial E}{\partial \hat{y}} \tag{6}$$

5.Steps 2-4 are repeated until the model runs for the set number of iterations:

$$v^{(k)} = v^{(k-1)} - \eta\nabla(k)v = v^{(k-1)} - \eta\frac{\partial E}{\partial v}, b_2^{(k)} = b_2^{(k-1)} - \eta\frac{\partial E}{\partial b_2} \tag{7}$$

$$w^{(k)} = w^{(k-1)} - \eta\nabla(k)w = w^{(k-1)} - \eta\frac{\partial E}{\partial w}, b_1^{(k)} = b_1^{(k-1)} - \eta\frac{\partial E}{\partial b_1} \tag{8}$$

2.3 Neural network prediction model

The prediction model of supercritical water gasification is composed of input layer, hidden layer and output layer in this paper. The hidden layer contains more layer structures.
The neural network will have a powerful spatial calculation and expression ability with many neurons in hidden layers, but too many hidden layers will waste computer resources and reduce the efficiency of model operation. The number of hidden layers in this paper is set as 2. The first hidden layer is set to 10 neurons while the second one is set to 6 neurons. In this way, the loss value is small and the efficiency of model operation is high at the same

time according to Table 1. The number of single hidden layer neurons is set to 10 in order to contrast with the model of double hidden layer. And the neural network structure diagram is shown in Figure 1.

The activation function brings a crucial nonlinear factor to the neural network, and the choice of the activation function has a great influence on the performance and convergence speed of the neural network model according to Ertuğrul (2018). As the activation function most frequently used in deep neural network learning, ReLU activation function is used in this paper due to its two characteristics, as follows. (1) The whole process can save a lot of computing resources and improve the efficiency of model operation due to the simple and fast calculation. (2) ReLU function can reduce the highly dependent relationship between parameters and alleviate the occurrence of over-fitting problems according to Pesch (2022).

The parameter optimiser in the model is set to Adam optimiser, and the learning rate of each parameter can be adjusted automatically and dynamically. Each iteration of the learning rate will have a certain range, and when the first-moment estimation of the gradient is used, the parameter adjustment can be carried out smoothly.

The loss function is set to MSE loss in terms of gradient solution and convergence calculation. This function curve can achieve rapid convergence, and the data used in this paper has no discrete value influence and avoid the effect of the outliers in the input data.

Table 1: Loss value of different neural network structures

Number of neurons in the first layer	Number of neurons in the second layer	MSE loss
8	6	10.35
10	6	6.70
12	6	4.74
15	6	12.45
10	0	60.10

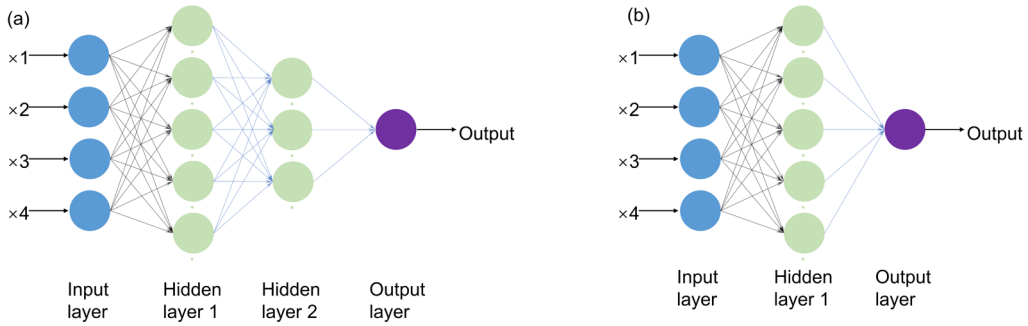

Figure 1: The structure of (a) A double hidden layer neural network model; (b) A single hidden layer neural network model

2.4 Evaluation index

Root mean square error (RMSE), coefficient of determination (R^2), and mean absolute error (MAE) are used to predict and evaluate the regression results of this model. The calculation equations are as follows:

$$RMSE = \sqrt{\frac{1}{n}\sum\left(y - y_{predict}\right)^2} \tag{9}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y - y_{\text{predict}})^2}{\sum_{i=1}^{n}(y - \frac{1}{n}\sum_{i=1}^{n} y)^2} \tag{10}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|(y - y_{predict})\right| \quad (11)$$

3. Results and discussion

3.1 Analysis of model prediction results

The reaction temperature, residence time, feedstock concentration and pressure are the main factors affecting the gasification process. Results at each condition are repeated three times and the average values are calculated to reduce the uncertainties. The value of these factors, obtained from the experiment, are inputted into the model as the characteristic value. 60 % of the data is inputted into the model for training. After this process, the carbon vaporisation rate, hydrogen vaporisation rate, hydrogen gas yield and total gas yield are obtained. RMSE, R^2, and MAE are calculated in order to analyse and evaluate the accuracy of the model accurately. The CPU time of double hidden layer model is about 13 min while that of single hidden layer model is about 6.2 min.

3.2 Comparison of training value and predicted value of double hidden layer

The results show that the conversion rates of both carbon and hydrogen, and the total gas yield have good prediction effects in this model. Among them, R^2 of carbon gasification rate and the total gas yield is 0.98, higher than that of the hydrogen gasification rate which equals 0.96. The results of hydrogen yield are not ideal, whose R^2 is 0.76, RMSE is 1.47, and MAE is 1.13.

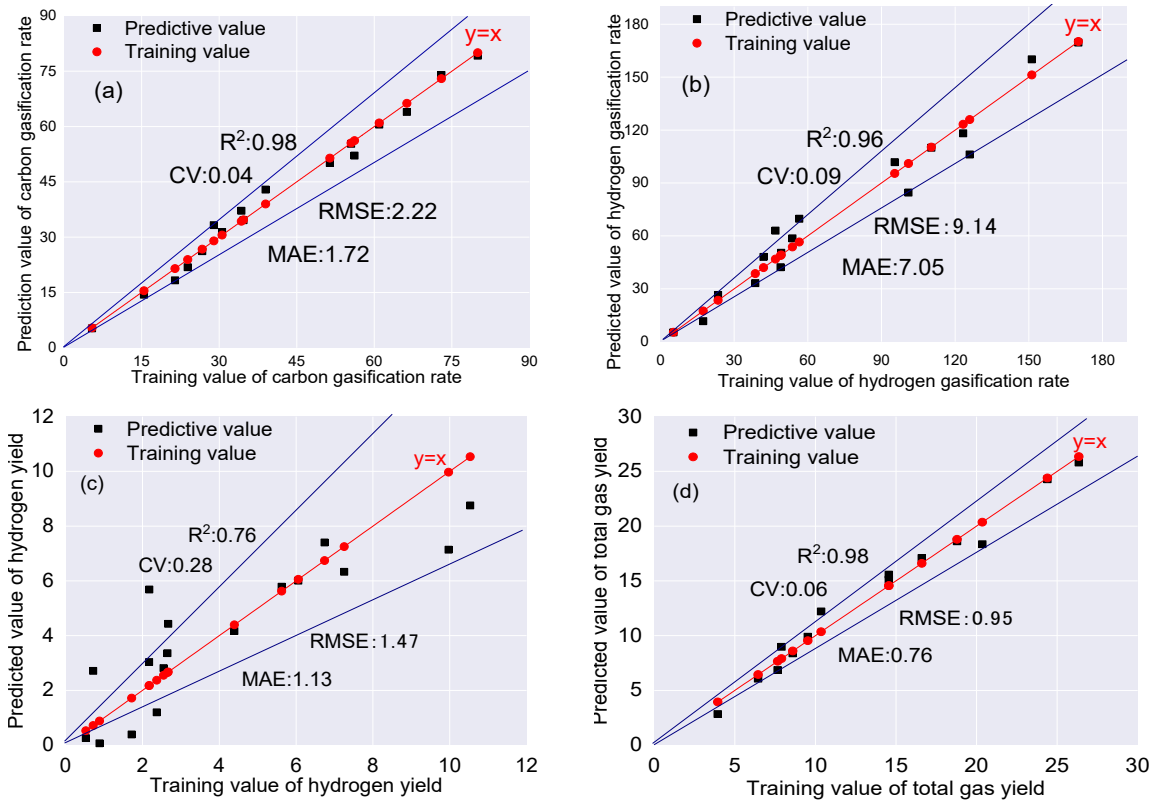

Figure 2: Correlation diagram between the predicted value and training value (a) Carbon gasification rate; (b) Hydrogen gasification rate; (c) Hydrogen yield; (d) Total gas yield

As shown in Figure 2, the predicted dispersion of hydrogen yield is relatively high, because the selected characteristic value is greater than the value of the hydrogen gas yield and local optimisation or even overfitting happens.

3.3 Comparison of training value and experiment data of double hidden layer

The experimental value of the carbon conversion rate still obtains the best prediction effect in this model, whose R^2 is 0.96, RMSE is 3.71, and MAE is 2.76. The prediction results of both hydrogen conversion rate and total gas

yield are also good, whose R^2 is above 0.91, RMSE is 11.5 and 1.83, and MAE is 9.28 and 1.39. The prediction results of hydrogen yield are also not ideal, whose R^2 is 0.75, RMSE is 1.29 and MAE is 1.02. The predicted value of hydrogen gas yield has a relatively high degree of dispersion as shown in Figure 3.

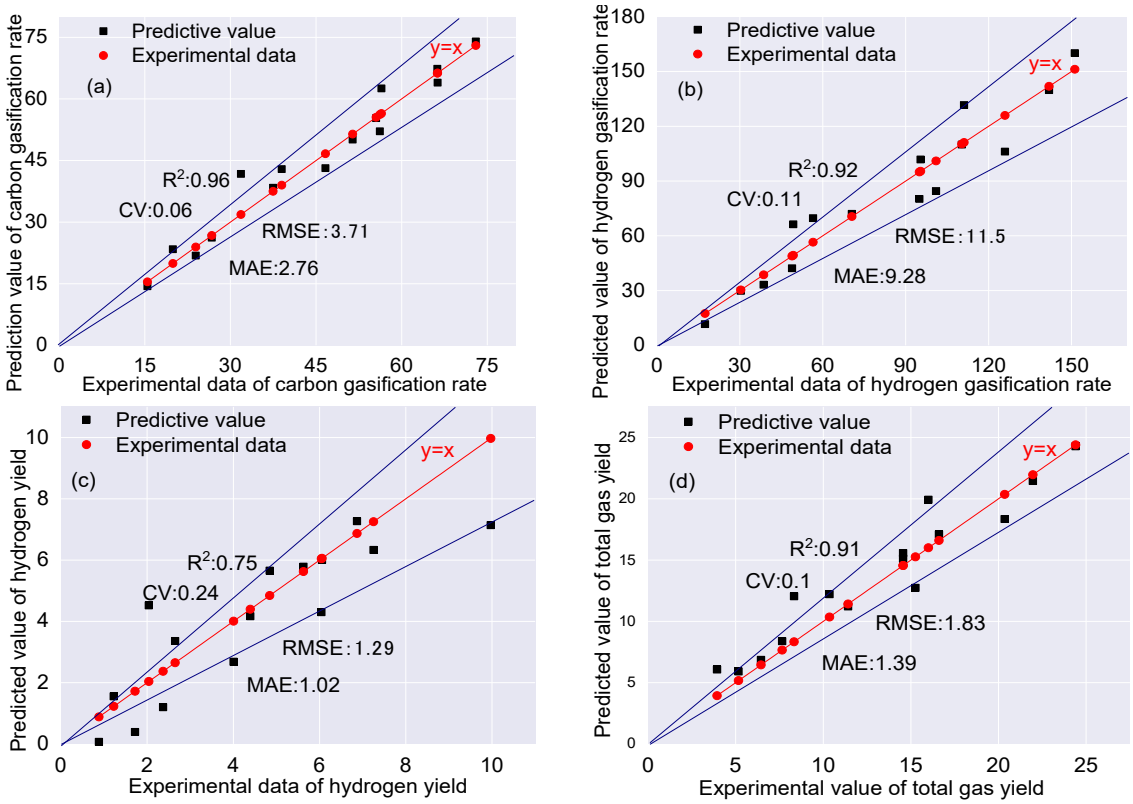

Figure 3: Correlation diagram between the predicted value and experiment data (a) Carbon gasification rate; (b) Hydrogen gasification rate; (c) Hydrogen yield; (d) Total gas yield

3.4 Results of single hidden layer model

The prediction results of hydrogen and carbon dioxide are not ideal and the loss function values derived from the program are shown in Table 2:

Table 2: Loss function values of different gasification products

	Carbon gasification rate	Hydrogen gasification rate	Hydrogen gas yield	Total gas yield
MSE	7.1355	83.613	2.2155	2.389

The loss value of hydrogen yield in loss function is 2.2155, and the value calculated by predicted data are also very close. Because the model runs into local optimisation due to the high model complexity. And the constructed single hidden layer neural network is used to simplify this model.

The prediction of hydrogen yield is better than that in a double hidden layer. Compared with the double hidden layer model, R^2 in a single hidden layer model increased by 10 % and it is 0.85. RMSE is 1.16, reduced by 13 %. MAE is 0.81, reduced by 21 %.

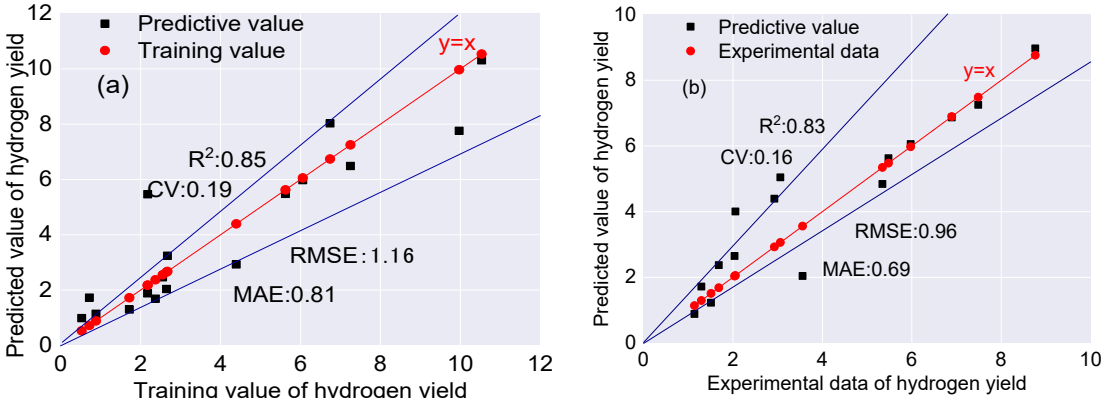

Figure 4: Correlation diagram of single hidden layer (a) Between predict value and training value; (b) Between predict value and experimental data

4. Conclusions

This paper uses the gasification data as a learning sample, a gasification artificial neural network model for waste circuit boards is constructed. This work aims to provide theoretical guidance for optimising reactor design and scale-up. Compared with the traditional model, this model has good performance, including accuracy and generality, and it can calculate fast with ReLU activation function. The simulation results of the proposed neural network model are in good agreement with the experimental data, as follows:

1. A double hidden layer neural network model is suitable for the prediction and analysis of the conversion rates of carbon and hydrogen. And the prediction of total gas yield can reach high accuracy.
2. The prediction of the hydrogen yield is not as accurate as that of other variables due to local optimisation, whose R^2 is 0.76, RMSE is 1.47 and MAE is 1.13.
3. A single hidden layer neural network model is used for the prediction of hydrogen yield. R^2 is 0.85 RMSE is 1.16, and MAE is 0.81.

However, intermediates are not considered in this paper and the process of gasification is out of sight. In future work, a more comprehensive model will be established with intermediate reactions so that intermediates can be considered.

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