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Research on C4 Olefins Prepared by Ethanol Coupling Based on BP Neural Network

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Abstract: *In order to analyze the effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity, BP neural network was trained to predict ethanol conversion and C4 olefin selectivity. Then, using the control variable method, the ethanol conversion and C4 olefin selectivity were predicted by neural network. Finally, the xgboost model is trained according to the data, and the particle swarm optimization algorithm is used to optimize the xgboost parameters in the training process, so that the prediction accuracy is improved from 65.97% to 93.75%, and the prediction accuracy is improved by 27.28%. Using the trained xgboost model to input the combination of different characteristic indexes, the final result is more than 350 degrees, and the optimal C4 olefin yield is 27.823%. The final result is that the yield of C4 olefin is 177.252%.*

Keywords: *control variable, BP neural network, Xgboost based on particle swarm optimization*

1. Introduction

C4 olefins are widely used in the production of chemical products and medicine. Ethanol is the raw material for the production of C4 olefins. During the preparation process, the catalyst combination (i.e. the combination of CO loading, Co / SiO2 and HAP loading ratio, ethanol concentration) and temperature will have an impact on the selectivity of C4 olefins and C4 olefin yield [1]. Therefore, it is of great significance and value to explore the process conditions for the preparation of C4 olefins by ethanol catalytic coupling through the combination design of catalysts [2].

2. BP Neural Network Regression Model

2.1. Problem analysis

It is necessary to analyze the effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity. This topic requires the analysis of different catalyst combinations. Therefore, we divide the whole catalyst combination into five indexes, namely, loading mode, CO loading, Co / SiO2 and HAP loading ratio, Co / SiO2 and hap mass and concentration, and ethanol concentration [3]. At this time, we have six indexes together with temperature. We used the control variable method to study the effects of these six indexes on ethanol conversion and C4 olefin selectivity. The data in Annex I makes the research results more reliable. We train the BP neural network model regression prediction model through the data in the table. Based on this model, the catalyst indexes given in the table are redistributed as input data, and the trained neural network gives the ethanol conversion and C4 olefin selectivity, then, the influence of an index on ethanol conversion and C4 olefin selectivity was analyzed by drawing according to the control variable method. [1]

2.2. Establishment of BP neural network regression model

BP neural network can be used to find the accurate functional relationship between input variables and output variables. The training process of neural network is to continuously update the existing input data, calculate the output each time, and compare it with the expected output. If there is an error, calculate the same error unit, and modify its own weight and threshold, finally, an exact functional relationship can be formed. The training process is divided into two steps:

(1) Forward propagation.

We input variables in the input layer. In this question, we determine the six indicators: loading mode,

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CO load, Co / SiO2 and HAP loading ratio, Co / SiO2 and HAP mass sum, ethanol concentration and temperature. The output layer is the variable we want to output. In this question, it has different effects on ethanol conversion and C4 hydrocarbon selectivity. The connection strength is the connection strength between the two nodes. These parameters are constantly modified in the process of training. The data input from the input layer will enter the hidden layer after weighted by the connection strength. The input of the hidden layer is:

$$h_{l1} = x_1 \cdot p_{11} + x_2 \cdot p_{21} + x_3 \cdot p_{31}. \tag{1}$$

The input is the weighted sum of each index and connection strength, and the output is the sigmoid function about the input. The sigmoid function is the stimulation function of neural network, which will normalize the weighted sum of input variables to ensure the normal training.

$$h_{o1} = \text{Sigmoid}(h_{l1}). \tag{2}$$

The process from hidden layer to output layer also conforms to the above principle.

$$y_i = h_1 \cdot q_{11} + h_2 \cdot q_{21} \tag{3}$$

$$y_o = \text{Sigmoid}(y_i) \ . \tag{4}$$

The output of a variable represents the completion of a forward propagation, followed by a back propagation.

(2) Back propagation.

Back propagation is the error between the expected y value and the network output y value. The error is usually expressed as a loss function.

$$E_p = \frac{1}{2}(y_0 - \text{y})^2 \ . \tag{5}$$

Then, the network adjusts the connection strength Q and threshold between the hidden layer and the output layer to make the error continue to decline along the gradient.

After repeated learning, the trained neural network can give a good relationship between input variables and output variables. It can process similar sample input information and give the results.

2.3. Solution of control variable model based on Neural Network

In matlab software, 20 groups of experimental data in Annex I were used for neural network training, in which the catalyst combination was divided into four indexes: CO load, Co / SiO2 and HAP loading ratio, Co / SiO2 and HAP mass and concentration, and ethanol concentration. There are five temperature indicators attached.

The effects of five indexes on ethanol conversion and C4 olefin selectivity were studied

Therefore, the input layer of neural network includes five indexes: CO load, Co / SiO2 and HAP loading ratio, Co / SiO2 and HAP quality and, ethanol concentration and temperature. The output layers are ethanol conversion and C4 olefin selectivity, respectively.

The prediction accuracy of neural network whose output variable is ethanol conversion is as follows:

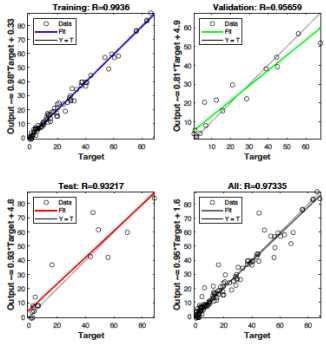

Figure 1: Accuracy test of BP neural network for ethanol conversion.

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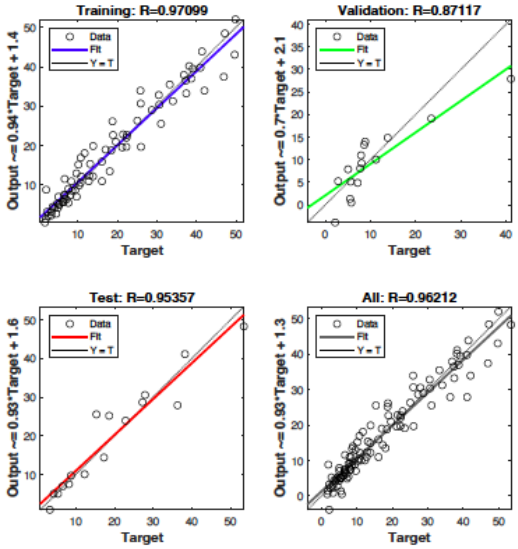

Figure 2: Accuracy test of C4 olefin selective BP neural network.

It is found that the trained neural network can well determine the relationship between input variables and output variables. The results given by neural network are reliable and the model test is passed.

Then, the experiments with different parameters were simulated by controlling variable method, and the effects of each index on ethanol conversion and C4 olefin selectivity were analyzed. [2]

3. Xgboost prediction model based on Particle Swarm Optimization optimization

3.1. Problem analysis

According to the analysis, two problems need to be solved. The first problem is to analyze how to select the catalyst combination and temperature to make the C4 olefin yield as high as possible under the same experimental conditions. The second problem is how to select the catalyst combination and temperature to make the C4 olefin yield as high as possible when the temperature is lower than 350℃. It can be found that the goals of the two problems are the same, but problem 2 has more conditions that the temperature is less than 350 degrees than problem 1. It can be seen from the appendix that the yield of C4 olefins depends on the ethanol conversion and C4 olefin selectivity. Therefore, firstly, calculate the C4 olefin yield of the corresponding experiment according to the data in Annex I. This problem is an optimization problem. We need to find out the optimal catalyst combination and temperature. We can train the xgboost model according to the selected indexes in the second question and the calculated corresponding C4 olefin yield. In the training process, the ant colony algorithm is used to adjust the xgboost parameters, so that it can realize the accurate regression prediction of C4 olefin yield. On the trained model, we can traverse the combination of indicators, and then find the optimal catalyst combination and temperature.

3.2. Xgboost prediction model based on Particle Swarm Optimization optimization

Xgboost is one of the boosting algorithms. The idea of boosting algorithm is that many weak classifiers are integrated to form a strong classifier. Because xgboost is a lifting tree model, it integrates many tree models to form a strong classifier.

3.2.1. Xgboost objective function

For the training set $T = \{(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)\}$, the loss function $l(y_i, \hat{y}_i)$, regularization term $\Omega(f_k)$.

Then the overall objective function is:

$$L(\emptyset) = \sum_i l(y_i, \hat{y}_i) + \sum_k \Omega(f_k). \quad (6)$$

Where $L(\emptyset)$ is the expression in linear space, I is the ith sample, K is the kth tree, $\hat{y}_i$ is the

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predicted value of the ith sample x_i.

Using gbdt gradient lifting tree expression xgboost.

Then $L(\emptyset)$ is converted into the following formula:

$$L(t) = \sum_i^n l\left(y_i, \hat{y}_i + f_t(x_i)\right) + \sum_k \Omega(f_k). \quad (7)$$

Optimize the objective function

After the second-order Taylor expansion and regularization expansion, the constant term is removed, and the primary term coefficients and secondary term coefficients are combined, the objective function is simplified as follows:

$$L(t) = \sum_{j=1}^T \left[G_j\omega_j + \frac{1}{2}\left(H_j + \lambda\right)\omega_j^2\right] + \gamma T. \quad (8)$$

Where G_j is the cumulative sum of the first-order partial derivatives of the samples contained in leaf node j, which is a constant, and H_j is the cumulative sum of the second-order partial derivatives contained in leaf node j, which is a constant.

3.2.2. Xgboost objective function

The objective formulas of each leaf node of the xgboost objective function are independent of each other, that is, the formula of each leaf node reaches the maximum point, and the whole objective function also reaches the maximum point.

The weight of each leaf node ω_j and reach the optimal obj target value at this time:

$$\omega_j = -\frac{G_j}{H_j+\lambda}. \quad (9)$$

$$Obj = -\frac{1}{2} + \sum_{j=1}^T \frac{G_j^2}{H_j+\lambda} + \gamma T. \quad (10)$$

3.3. Particle swarm optimization

The steps of particle swarm optimization algorithm are given

(1) Firstly, initialize a particle swarm, including the initial position of the particle, the velocity of the particle, the inertia factor of the example, etc

(2) Calculate the initial fitness value of each particle

(3) Take the initial fitness value of all particles as the local optimal value of each particle, save it, find the optimal value, take it as the initial value of the global optimal value, and record the position.

(4) Updates the speed and position of each particle.

(5) Calculate the fitness value of the updated particles, update the local optimal value of each particle and the global optimal value of the whole particle swarm.

(6) Repeat 4-5 until the iteration end condition is met. [3]

3.4. Optimal value search

Based on the input data set of xgboost model, the final result is that the yield of C4 olefins is the best 27.823% when the temperature is greater than 350 degrees, and the final result is that the yield of C4 olefins is the best 177.252% when the temperature is less than 350 degrees.

References

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