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Research on Catalyst Combination for Ethanol Coupling Preparation of C4 Olefins Based on BP Neural Network

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Abstract: In this paper, a grey correlation analysis model based on BP neural network is established for the preparation of C4 olefins by ethanol coupling. Firstly, the grey correlation analysis of ethanol conversion, C4 olefin selectivity and its influencing factors was carried out, and the correlation degree of 5 factors in the catalyst combination was obtained. Then, the BP neural network structure is constructed to predict the obtained correlation degree. It is concluded that the average relative error between the calculated correlation degree and the predicted correlation degree is 1.7%, which verifies the rationality of the model. Finally, the residual analysis of the results shows that the absolute error is 5.3%.

1. Introduction

With the further development of chemical and energy industries and the further upgrading of production capacity, the preparation of C4 olefins is of key significance. The further increase in the output of ethanol promotes the further improvement of the requirements for the process of ethanol blending C4 olefins. The process of preparing C4 olefins from ethanol needs a catalytic process. The selection of catalyst and the control of catalytic temperature have a great impact on the selectivity and yield of C4 olefins. This paper mainly discusses the effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity.

2. Model Establishment and Solution

2.1 catalyst combination influence model based on grey correlation analysis

(1) Determine analysis sequence

Different catalyst combinations have different effects, among which four factors play a major role, namely, CO loading, Co / SiO2 content, HAP content and ethanol concentration. These four indexes replace the five independent variables of catalyst combination and temperature composition. Ethanol conversion and C4 olefin selectivity are two dependent variables. The data is deeply mined and analyzed, and rearranged into a table according to these seven indicators. Take the serial number as the reference sequence and each index as the comparison sequence.

(2) Dimensionless of variables

1) The initial value processing can dimensionless process the data:

$$x_i(k) = \frac{x_i(k)}{x_i(1)}, k = 1, 2, 3, ..., n; i = 1, 2, 3, ..., m$$

2) Averaging can also process the data dimensionless:

$$x_i(k) = \frac{x_i(k)}{\overline{x}_i}, k = 1, 2, 3, ..., n; i = 1, 2, 3, ..., m$$

Where, i represents a row corresponding to the comparison sequence, and k represents each index. Because the magnitude of the sequence of the same factor is quite different, the mean processing is used to make the variables dimensionless.

(3) Calculate correlation coefficient

The correlation coefficient is the correlation degree value of each index between the comparison series and the reference series. The reference sequence after data processing is: $x_i' = (x_i'(1), x_i'(2), x_i'(3), \cdots x_i'(k), \cdots x_i'(n))$

The comparison sequence is as follows:

$$x_i' = (x_i'(1), x_i'(2), x_i'(3), \cdots x_i'(k), \cdots x_i'(n)), \quad i = 1, 2, ..., m$$

The correlation coefficient is:

$$\zeta_i(k) = \frac{\min_i \min_k |x_0(k) - x_i(k)| + \rho \cdot \max_i \max_k |x_0(k) - x_i(k)|}{|x_0(k) - x_i(k)| + \rho \cdot \max_i \max_k |x_0(k) - x_i(k)|}$$

Where, $\min_i \min_k |x_0(k) - x_i(k)|$ represents the two-stage minimum value, $\max_i \max_k |x_0(k) - x_i(k)|$ represents the two-stage maximum value, ρ is the resolution coefficient, and its value range is (0 to infinity). The smaller ρ, the greater the resolution, usually 0.5.

(4) Calculate correlation

Since there are more than one correlation coefficient obtained in the previous step, and the information is too scattered, it is difficult to make an overall comparison. Therefore, it is necessary to concentrate the correlation coefficient of each index into one value as a quantitative representation of the correlation degree between the comparison series and the reference series. After calculation, the average value is good.

$$r_i = \frac{1}{n} \sum_{k=1}^{n} \xi_i(k), k = 1, 2, \cdots, n$$

(5) Relevance ranking

The correlation degree is sorted by size. If $r_1 < r_2$, the reference sequence y is more similar to the comparison sequence x_2.

2.2 Optimization Model Based on BP Neural Network

The correlation degree between the parameters of the catalyst and ethanol conversion and C4 olefin selectivity was obtained by grey correlation analysis, and the correlation degree was optimized by BP neural network. BP neural network consists of output layer, input layer and hidden layer. The input layer includes co loading, Co / SiO2 content, HAP content, ethanol concentration and temperature, and the output layer includes ethanol conversion and C4 olefin selectivity. The number of input layer nodes is 5, the number of hidden layer nodes is 5, the number of output layer nodes is 1, and the neural network structure is 5-5-2

The error of BP neural network is evaluated by correlation coefficient, average relative error and root mean square error.

Correlation Coefficient: $r = \frac{cov(a,p)}{\sqrt{cov(a,a)cov(p,p)}}$

Average Relative Error: $MRE(\%) = \frac{1}{M}\sum_{i=1}^{M}\left|100\frac{d_o - y_o}{y_o}\right|$

Root Mean Square Error: $RMSE = \sqrt{\frac{1}{M}\sum_{i=1}^{M}\left(\frac{d_o - y_o}{y_o}\right)^2}$

2.3 Model Solving Process

2.3.1 Solution of grey correlation analysis model

Firstly, the data were processed, and the parameters of 114 groups of experimental catalyst combinations were obtained by splitting each group of catalyst combinations according to four indexes: CO loading, Co / SiO2 content, HAP content and ethanol concentration. The five indexes of CO loading, Co / SiO2 content, HAP content, ethanol concentration and temperature were treated dimensionless to obtain the parameter values of each catalyst combination.

Then, calculate the correlation coefficient between the five indexes and ethanol conversion, and then calculate the correlation degree of the five indexes on ethanol conversion and C4 olefin selectivity, and obtain the following table:

Table 1: Correlation degree of each index

evaluating indicator	Correlation degree of ethanol conversion	C4 olefin selectivity correlation
Co load	0.913	0.937
Co / SiO2 content	0.917	0.943
HAP content	0.917	0.942
Ethanol concentration	0.914	0.939
temperature	0.395	0.404

Table 2: Ranking results of correlation degree

Evaluation item	ranking
Co load	4
Co / SiO2 content	1
HAP content	2
Ethanol concentration	3
temperature	5

It can be concluded from the above table that temperature has little correlation with ethanol conversion and C4 olefin selectivity. Therefore, it can be analyzed that temperature has little impact on C4 olefin yield, and the high temperature resistance of the reaction process is good. However, the correlation value of CO load, Co / SiO2 content, hap content and ethanol concentration on ethanol conversion and C4 olefin selectivity reaches 0.9, these indicators have a great impact on ethanol conversion and C4 olefin selectivity. Therefore, in the reaction process, CO loading, Co / SiO2 content, HAP content and ethanol concentration need to be controlled to some extent, otherwise, the yield of C4 olefins will be affected.

Finally, the obtained correlation degree is sorted to obtain the sorting results shown in the following table.

It can be seen from the above table that temperature has the least correlation with ethanol conversion and C4 olefin selectivity, and temperature has little effect on ethanol conversion and C4 olefin selectivity; Co loading, Co / SiO2 content, HAP content and ethanol concentration have great effects on ethanol conversion and C4 olefin selectivity.

2.3.2 Solution of BP neural network

The independent variables are co loading, Co / SiO2 content, HAP content and ethanol concentration. The dependent variables are 114 data of ethanol conversion and C4 olefin selectivity as samples, and the first 79 groups of data as training samples to train the model. The last 35 samples are used as test samples to test the model.

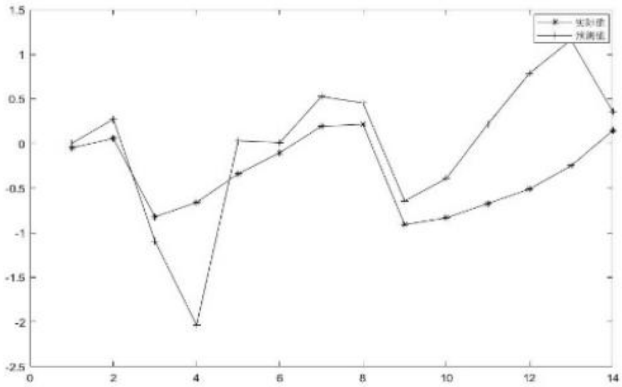

Figure 1: BP neural network error analysis of C4 olefin selection rate

As shown in Figure 1, the error curve between the actual value and the predicted value is obtained after the ethanol conversion and C4 olefin selectivity are predicted by BP neural network. Obviously, it can be seen from the figure that with the increase of the number of samples, the actual value and the predicted value are getting closer and closer in the overall trend, indicating that the simulation results of neural network are gradually close to the actual value with the increase of the number of iterations. When it is near sample 6, the minimum error is 0.2.

3. Model Evaluation

In this paper, grey correlation analysis is used to evaluate multiple objects at the same time, but it can only judge the existing optimal scheme, and can not get the optimal scheme. In the follow-up, we can continue to conduct in-depth research on the catalyst combination and temperature in the chemical reaction, which has significantly improved the temperature control and catalyst combination allocation in the chemical industry, so as to make the chemical reaction as full as possible, improve the efficiency and reduce the residue.

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