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Neural Network Model for Preparation of C4 Olefins by Coupling Ethanol

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Abstract

In the field of chemical production, it is important to prepare C4 olefins by coupling ethanol. During this process, the selectivity and yield of C4 olefins are affected by catalyst's combinations, temperature and time. It is significant for production, environmental protection and other aspects to study how to select catalyst combinations and temperature to make the yield of C4 olefins as high as possible under the same experimental conditions. By aiming at the process of preparing C4 olefins from ethanol production, and using the basic knowledge of optimization model and neural network, this paper establishes a mathematical model which explores how to select catalyst combination and temperature. The model is under the condition when the C4 olefin yield is as high as possible from the perspective of catalyst combination, temperature , time , and C4 olefin yield.

Keywords

Ethanol Coupling; Optimization Model; Neural Network Model.

1. Research Background

The method of preparing C4 olefins by ethanol coupling is very common in chemical production. The two factors closely related to its yield and efficiency are the selectivity of C4 olefins and the yield of C4 olefins, which are the proportion and reaction rate of C4 olefins in all products. Higher selectivity and yield undoubtedly mean lower cost and higher income. Therefore, it is of great significance to study the scheme with the highest C4 olefin yield under certain variables for production investment, environmental protection and cost reduction.

In order to make a thorough injury into the best process conditions for the preparation of C4 olefins by ethanol coupling, it is necessary to understand the dependent variables and independent variables in the preparation process. According to a series of experimental performance data sheets of a chemical laboratory under different catalysts and temperatures, as well as the test data of a given catalyst combination at 350 °C, we know that common catalyst combinations include the combination of CO loading, Co / SiO2 and HAP loading ratio and ethanol concentration. And when the temperature is 350 °C, the conversion of ethanol and the selectivity of the product change with time under certain conditions of the catalyst.

We introduce the concept of C4 olefin yield which is equal to the conversion of ethanol multiplied by the selectivity of C4 olefins to make the production efficiency of C4 olefins more intuitive. Considering that there are multiple independent variables and one dependent variable, we use neural network model to solve this problem. After several iterations, the parameters processed by the neural network model are close to the predicted value, and three iterations are adopted here. After comparing the goodness of fit, we take 54 groups of data from A1 to A10 as the training set and 20 groups of data from a11 to A14 as the test set. After the trained network is substituted into the verification set to verify the a11 to A14 data, we can predict the C4 olefin yield in the data range.

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After analyzing the above data, in order to better reduce the industrial production cost and improve the efficiency and C4 yield, we designed experiments respectively at the temperature of 250 °C, 275 °C, 300 °C, 325 °C and 400 °C , to test the conversion of ethanol and the selectivity of ethylene, c4 olefins , acetaldehyde and other products under the same catalyst combination.

2. Structure of Neural Network Model

2.1. Building of BP Neural Network Model

According to the performance data obtained from the chemical laboratory, the process of ethanol coupling to prepare C4 olefins is very complex. Facing multiple independent variables and two dependent variables, the BP neural network model can efficiently predict under which conditions C4 olefin yield is the highest. We use the uniformly distributed random number to set each weight to a small random number, input the training data to one of the input data in [x (k), D (k)], and calculate the error of the output layer:

$$\begin{aligned} e_j(k) &= d_j(k) - y_j(k) \\ \delta_j(k) &= e_j(k) f'\left[S_j(k)\right] \end{aligned} \tag{1}$$

Then use equation 1-2 to calculate the error of the middle layer:

$$\begin{aligned} e_h(k) &= \sum_l W_{hl}(k)\delta_l(k) \\ \delta_h(k) &= e_h(k) f'[S_h(k)] \end{aligned} \tag{2}$$

The h is a node on the same level, H is the number of nodes in the middle layer, and l is the next layer of all nodes in the middle layer node. Update the weight of the network:

$$W_{pq}(k+1) = W_{pq}(k) + \eta\delta_q(k) y_p(k) \tag{3}$$

The A is the weight of the middle layer node P or the input p to Q, and Q is the output of node P or the input of node Q.

The process of iteration is the process of back propagation. After iteration, the parameters are more and more similar to our prediction. However, as the network begins to over match the training data, the error of the validation data set may begin to increase, so we used three iterations to predict the optimal process conditions.

We use Matlab to write the BP neural network algorithm program, which contains three layers of network, each layer has 15 hidden layer neurons and one output neural node, as shown in Figure 1.

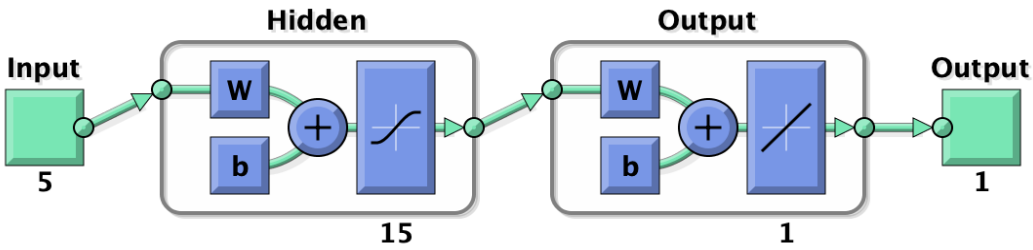

Figure 1. Program diagram of BP neural network algorithm

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We take 54 sets of data from A1 to A10 as training sets, and A11 to A14 as 20 sets of data as test sets. After adjusting the number of hidden layer neurons, training times and the upper limit of training error for many times, the goodness of fit of our model reaches 0.9876, which is relatively satisfactory. As shown in Figure 2, although there is a certain deviation between the sample value and the check value, the change trend of C4 olefin yield is consistent. Therefore, it can be considered that the neural network model is trained by the sample set. In this way, we can use it to predict the C4 olefin yield in the data range.

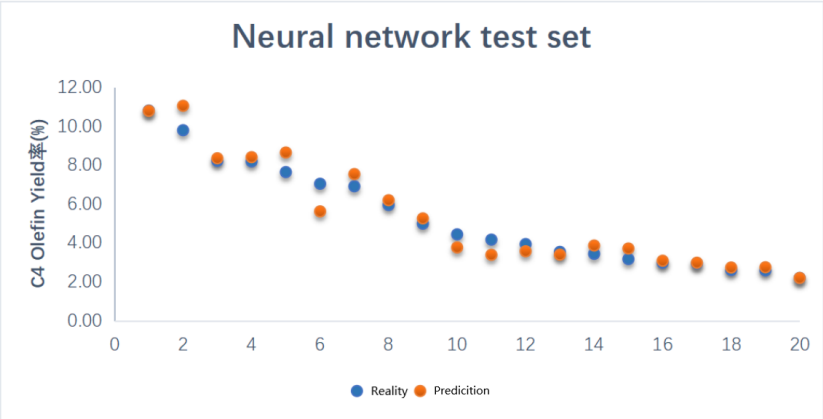

Figure 2. Comparison between actual and predicted C4 olefin yield

2.2. Data Analysis of Catalyst Combination and Unlimited Temperature

When discussing the selection of catalyst combination and temperature under two conditions of temperature ranging from 0 to 400 °C and 0 to 350 °C, by establishing a multiple linear regression model for the B feeding method, we obtained an ideal correlation result. The specific process is no longer explained here. The conclusion is given. The ethanol conversion rate is affected by temperature, Co/SiO2 and HAP charging ratio, and the temperature has a greater impact on the ethanol conversion rate especially. Under other conditions unchanged, the ethanol conversion rate can be increased by 0.28% for every 1°C increase, and the ethanol conversion rate can be increased by 0.07% for each additional 1 mg of Co/SiO2 and HAP loading. The conversion of C4 olefins also has a similar situation which is affected by temperature, Co/SiO2 and HAP charging ratio. Under other conditions unchanged, the conversion rate of C4 olefins can be increased by 0.89% for every 1°C increase, and the conversion rate of C4 olefins can be increased by 0.07% for each increase of 1 mg of Co/SiO2 and HAP loading. However, the higher temperature will cause a lot of energy waste. Therefore, we choose the highest temperature in the known experimental data, and then a large amount of random data is used to test the neural network model. After using multiple iterations, the groups with high yields were iteratively tested to improve the accuracy, and the 5 groups with the highest yields were finally taken out.

Table 1. The 5 groups with the highest yield and the corresponding process conditions

Yield	x1	x2	x3	x4	x5
73.3425	450.00	3.50	200.00	200.00	1.31
73.3423	450.00	3.50	200.00	200.00	1.30
73.3423	450.00	3.50	200.00	200.00	1.30
73.3414	450.00	3.50	200.00	200.00	1.32
73.3409	450.00	3.50	200.00	200.00	1.29

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According to the data in the Table 1, when the temperature is 450 °C, the catalyst combination is 200mg 3.5wt% Co/SiO2- 200mg HAP-ethanol concentration 1.30ml/min when the C4 olefin yield is the highest.

2.3. Data Analysis for Temperature Below 350°C

Similarly, through four iterations, five sets of data with the highest yield when the temperature is lower than 350 °C are obtained, as shown in Table 2.

Table 2. The 5 groups with the highest yield within 350°C and the corresponding process conditions

Yield	x1	x2	x3	x4	x5
37.6144	350.00	2.88	200.00	200.00	2.10
37.6121	350.00	2.86	200.00	200.00	2.10
37.6103	350.00	2.90	200.00	200.00	2.10
37.6103	350.00	2.90	200.00	200.00	2.10
37.6032	350.00	2.84	200.00	200.00	2.10

According to the data in the table, if the temperature is not higher than 350℃, the catalyst combination is 200mg 2.88wt% Co/SiO2-200mg HAP-ethanol concentration 2.10ml/min when the C4 olefin yield is the highest.

3. Optimization and Reason of Experiment

Temperature, catalyst and time are three important factors in chemical production and pharmaceutical processing. In order to improve the yield of C4 olefins in the preparation of C4 olefins by ethanol coupling, we should start from improving the rate of chemical reaction and the minimum time and temperature when the yield reaches the maximum yield. When the positive and negative reaction rates of the reversible reactions are equal, the equilibrium of chemical reaction at the surface is reached at the same time, and temperature becomes an important factor affecting the equilibrium state of this reversible reaction. Catalyst plays a key role in reducing reaction activation energy and increasing reaction rate in the preparation of C4 olefins by ethanol coupling. Time cost should also be considered in production, which is closely related to the competitiveness of factories or enterprises in the market. We have conducted experiments and discussions on the relationship between the three, there are catalyst determination, time determination, and discussion at different temperatures; temperature determination, time determination, and reaction comparisons under different catalyst combinations. In order to improve the original experiment, optimize the verification, and facilitate the production, we propose to increase the yield of C4 olefins at different times when the temperature is determined and the catalyst combination is the same to achieve the situation where the process conditions and raw materials are the same, the time cost is the smallest and the C4 olefin yield is the largest.

After modeling and analysis, the temperature conditions and catalyst combination conditions for the highest yield of C4 olefins are based on experiments at 250°C, 275°C, 300°C, 325°C, 400°C, and 450°C. Carrying out research at 450°C is contrary to the original intention of improving yield and reducing cost, and is also not conducive to actual industrial production. There is a relationship of succession and complementarity with the original experiment.

We have established five experimental tables to supplement the experiments, only one group is listed here (as shown in Table 3). Through BP neural network analysis, the correlation curve

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of the theoretical value of the experiment can be obtained, which can be used as a reference in chemical experiments. However, because there is no known data and there are only two independent variables, it is difficult to predict the data through Matlab.

Table 3. Experiment 1

Experiment 1: Test data for a given catalyst combination at 250°C							
Time (min)	Ethanol conversion(%)	Selectivity(%)					
		Ethylene selectivity	C4 olefin	Acetaldehyde	Fatty alcohol with 4-12 carbon atoms	Methylbenzaldehyde and methylbenzyl alcohol	other
20							
70							
110							
163							
197							
240							
273							

4. Popularization Significance and Disadvantage

The yield of C4 olefins is affected by many factors. After comprehensively considering various constraints, we selectively consider the optimal parameters within a certain range to ensure the rationality of the results and draw the conclusion: when the temperature is 450°C and the catalyst combination is 200mg 3.5wt% Co/SiO2- 200mg HAP-ethanol concentration 1.30ml/min, the C4 olefin yield is the highest; when the temperature is not higher than 350℃, the catalyst combination is 200mg 2.88wt% Co/SiO2- 200mg HAP-ethanol concentration 2.10ml/min, the C4 olefin yield is the highest. Since each manufacturer has different inputs for raw materials, equipment, etc., to find the optimal process conditions to improve profits and reduce costs, the established models and analysis methods are very meaningful.

However, other factors such as pressure, acidity and alkalinity will also exist in the actual preparation of C4 olefins. Since it only considers the effects of time, temperature, catalyst combination, and catalyst charging method, this model has certain limitations.

5. Conclusion

We used three iterations and four iterations of the BP neural network model to analyze the catalytic coupling of ethanol to prepare C4 olefins to improve the reliability of the data. The final conclusion is that when the temperature is 450°C and the catalyst combination is 200mg 3.5wt% Co/SiO2- 200mg HAP-ethanol concentration 1.30ml/min, the C4 olefin yield is the highest. When the temperature is not higher than 350℃, the catalyst combination is 200mg 2.88wt% Co/SiO2- 200mg HAP-ethanol concentration 2.10ml/min, the C4 olefin yield is the highest.On the basis of the original data, the discussion on the optimal yield of C4 olefins at

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different times in the same catalyst combination mode is supplemented, which improves the experiment and is closer to production, and has certain generalization.

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