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Study on Preparation of Ethanol-coupled Olefins Based on Neural Network Algorithm

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Abstract: To explore the process conditions for the preparation of C4 olefins by ethanol coupling is of great significance to better promote the production of pharmaceutical and chemical products, so this paper focuses on the problems under this background. Firstly, the radar diagrams of ethanol conversion and C4 olefin selectivity of various catalyst combinations at different temperatures are drawn by using Matlab software, and then based on the idea of backward propagation algorithm, neural network model I is established. The coefficients in the model were solved by Python, and the relationship between the temperature of each catalyst and ethanol conversion and C4 olefin selectivity was obtained. It is concluded that in order to achieve the highest selectivity of C4 olefins, the temperature should be controlled reasonably and the catalyst should be optimized.

1. Introduction

With the shortage of fossil energy and the aggravation of environmental pollution, the traditional method of using fossil raw materials to produce chemical products is gradually replaced by the method of catalyst combination design to prepare chemical products. C4 olefin is a widely used raw material in the production of pharmaceutical and chemical products[1]. Ethanol is needed to produce C4 olefin. In the process of production and preparation of C4 olefins, the yield and selectivity of C4 olefins will be affected by the choice of catalyst combination and temperature. Based on a series of experiments carried out in a chemical laboratory under different temperatures and different catalyst conditions, the corresponding results are obtained.

2. Data preprocessing

First of all, the process diagram of the chemical reaction is obtained.

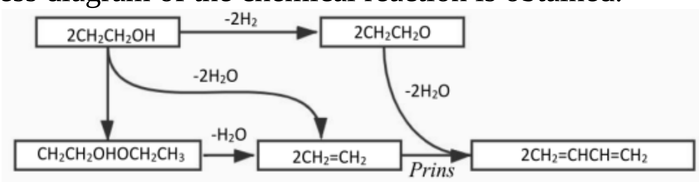

Figure 1: Process diagram of catalytic reaction

In order to quantitatively analyze the relationship between temperature and C4 olefin selectivity and ethanol conversion under the action of each catalyst, the collected experimental data were compared and analyzed. First of all, the radar diagrams of ethanol conversion of various catalyst combinations at different temperatures are drawn by MATLAB. It can be observed that both catalyst combinations and temperature have effects on ethanol conversion, and the effects are different.

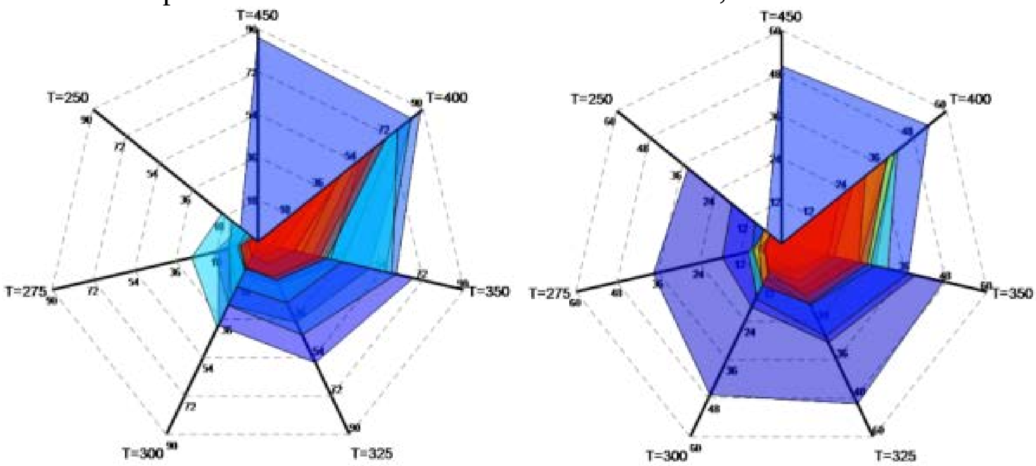

Figure 2: Radar group diagram of ethanol conversion and C4 olefin selectivity of various catalyst combinations at different temperatures

Similarly, the radar chart of C4 olefin selectivity of various catalyst combinations at different temperatures can be drawn.

3. Process of catalytic coupling of ethanol to C4 olefins

Each ethanol molecule contains a hydroxyl group. In order to prepare olefins containing only hydrocarbon elements, alcohol organic compounds need to remove the hydroxyl group and form carbon carbon double bond. There are methyl benzaldehyde, methyl benzyl alcohol, acetaldehyde, ethylene and other products in the data. Combined with the principle of organic chemistry, it can be inferred that the products contain OH2 and other products.

Temperature and catalyst are important process conditions for the preparation of C4 olefins. Ethanol is the raw material of chemical reaction, while C4 olefins and ethylene are the products of chemical reaction. Selectivity represents the proportion of a product in all products, so the purpose of the experiment should be to ensure that the selectivity of C4 olefins is as large as possible, while the selectivity of other products such as ethylene and acetaldehyde is as small as possible. At the same time, in order to ensure the full utilization of raw materials, the conversion of ethanol should also be as high as possible. Combined with the test of each catalyst combination at different temperatures, the experiment is divided into group A and group B according to the different loading methods of the catalyst combination, and the experimental results are described together and compared and analyzed. The C4 olefin selectivity and ethanol conversion of 21 kinds of catalysts at different temperatures were plotted into a line chart by using Matlab software, and the performance data diagrams of each catalyst at different temperatures were obtained. After comparative analysis, the reaction data of 9 kinds of catalyst combinations which are the most representative of the 21 images are selected to display. Thirdly, the combination diagram of the performance data of the nine catalysts at different temperatures was drawn by Matlab software, and the changes of ethanol conversion and C4 olefin selectivity were further observed with the change of temperature, as shown in the following figure.

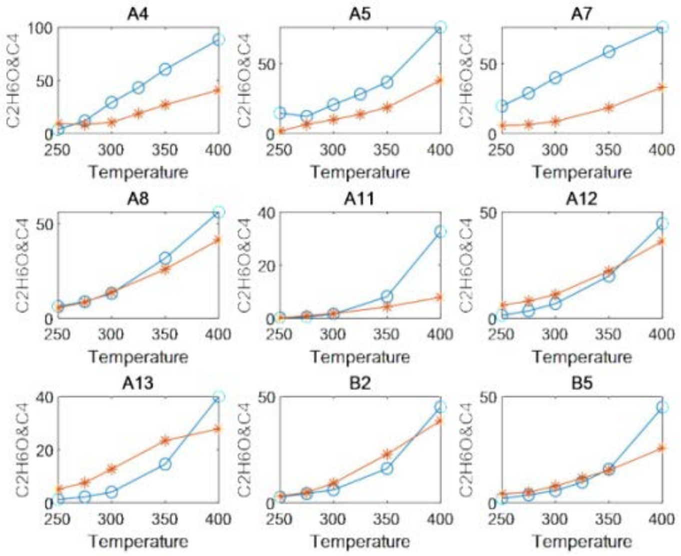

Figure 3: Combination diagram of performance data changes of nine representative catalysts at different temperatures

With the increase of temperature, the catalytic effect of each catalyst combination can be enhanced to a certain extent.

Based on the analysis of the relationship between the performance data of each catalyst and temperature, the effects of different temperatures on the conversion of ethanol and the selectivity of C4 olefins were discussed for each catalyst combination. In order to explore the effects of different temperatures on the conversion of ethanol and the selectivity of C4 olefins, for the convenience of calculation, the performance data of each catalyst at different temperatures are considered to be expressed in a more intuitive way.

The expression of the effect of each catalyst on ethanol conversion at different temperatures is expressed by matrix G. The expression $g_j(T)$ in line j represents the effect of temperature of catalyst combination j on ethanol conversion.

$$G = \begin{pmatrix} g_1(T) \\ g_2(T) \\ \vdots \\ g_j(T) \end{pmatrix}, \quad j = 1, 2, \cdots, 21 \tag{1}$$

The relationship between the temperature of each catalyst and the conversion of ethanol is expressed by matrix K. The following is an exploration of the preliminary judgment of figure 3. From fig. 3, we get the results that the effect of different catalyst combinations on the selectivity of C4 at different temperatures.

4. Neural network model

The neural network model consists of three parts: input layer, hidden layer and output layer[2][3]. The hidden layer may be composed of multiple layers. The number of hidden layers depends on the difference between ideal value and real value and the minimum value of absolute value. The input unit of the input layer is represented by x_1, x_2 the hidden unit of the hidden layer is represented by $a_1^{(j)}$,$a_2^{(j)}$, and the ideal value of the output layer is represented by $f^{(j)}(x)$. The hierarchical diagram of the neural network model is as follows

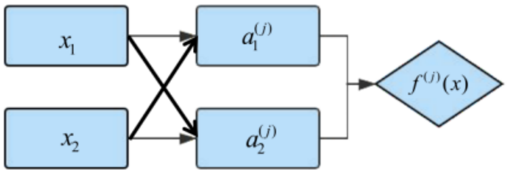

Figure 4: Neural network model hierarchy diagram

Establishment of neural network model I

$$\min[f^{(j)}(x)-f^{(j-1)}(x)]^2$$
$$\begin{cases} f^{(j)}(x)=w_1^{(j)}a_1^{(j-1)}+w_2^{(j)}a_2^{(j-1)} \\ \quad\quad\quad\quad\quad\quad\cdots \\ a_1^{(1)}=w_{11}^{(1)}x_1+w_{12}^{(1)}x_2 \\ a_2^{(1)}=w_{21}^{(1)}x_1+w_{22}^{(1)}x_2 \end{cases} \tag{2}$$

$a_1^{(j)}, a_2^{(j)}$ represents the hidden unit of the hidden layer, $f^{(j)}(x)$ represents the ideal value of the output layer, x_1 x_2 represents the input unit of the neural network input layer, and w represents the weight

5. Neural network model solving

Taking the catalyst combination A1 in the data as an example, the experimental data of A1 were extracted, and the thermal maps of temperature, product selectivity and ethanol conversion were drawn. The color of each small pixel block in the thermal map represents the correlation between the two variables of its corresponding coordinates. Red represents positive correlation, blue represents negative correlation, and the darker the color is, the stronger the correlation between variables is.

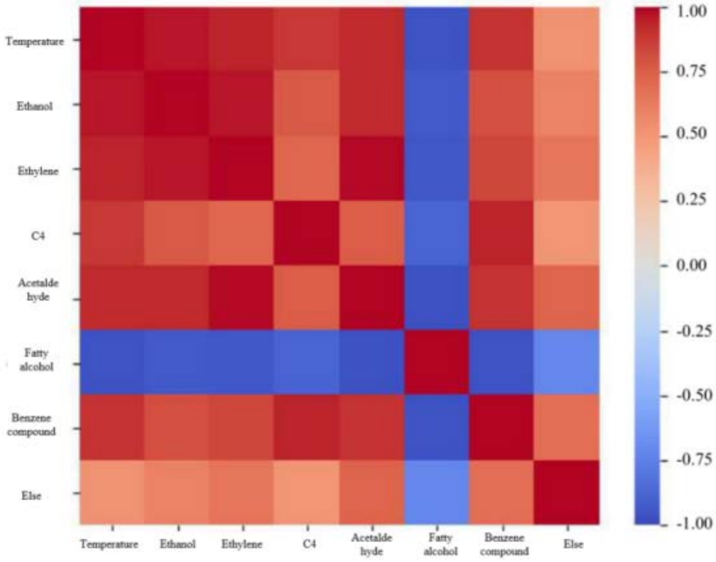

Figure 5: Thermodynamic diagram of correlation between temperature and selectivity of products and ethanol conversion

It can be seen from the thermodynamic diagram that taking catalyst combination A1 as an example, the pixel block colors of C4 olefin selectivity, ethanol conversion and temperature are dark red[4], indicating that there is a positive correlation between temperature and C4 olefin selectivity and ethanol conversion. At the same time, the pixel block color of ethanol conversion is darker than C4 olefins, indicating that temperature has a greater impact on ethanol conversion.

Take the temperature as the independent variable to make the model summary table, as shown in the following table

Table 1: Goodness of fit table of catalyst combination 1A

R	R^2	Adjust R^2	Standard error of estimate
0.992	0.983	0.978	0.167

In curve estimation, R square is the goodness of fit, which represents the fitting degree between the regression line and the observed value. Therefore, the closer r square is to 1, the better the fitting of the model can be proved. From the results in Table 1, the R-square obtained by calculating the value of R-square and the standard error of the estimated value is 0 983, which shows that the model fitting is very good.

6. Conclusion

In order to explore the process of ethanol coupling preparation of C4 olefins, the radar graphs of ethanol conversion and C4 olefin selectivity of various catalyst combinations at different temperatures were drawn by Matlab software, and the relationships between the temperature of each catalyst combination and ethanol conversion and C4 olefin selectivity were compared. Then the neural network model is established and the coefficient in the model is solved, and the relationship between the temperature of each catalyst and ethanol conversion and C4 olefin selectivity is obtained. Finally, it is concluded that the conversion of C4 olefin or ethanol can be the highest at the right temperature and optimizing the combination of catalysts.

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