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Study on the Optimum Process Conditions for Preparation of C4 Olefins by Ethanol Coupling

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Abstract: C4 olefins are widely used in industrial, medical and other important fields. The preparation of C4 olefins by ethanol coupling is an important research direction at present. In this paper, a mathematical model is established by BP neural network, the NetLogo simulation is designed, and the optimum process conditions for preparing C4 olefins by ethanol coupling is studied.

Keywords: Pearson correlation coefficient, Multiple regression model, BP neural network, NetLogo simulation.

1. Introduction

At present, China is in the era of rapid development, in which the rapid development of industry will play a greater role in promoting the economy. As a raw material of industry, C4 olefins are widely used in industry, medical treatment, military and other fields, and play a very important role in promoting the economic development of China. In order to further promote the development of industry, it is of great significance to study the preparation of C4 olefins.

The research of Chinese scholar Hongtao Wang et al. [1] [2] [3] provided a coupling method of C4 olefins catalytic cracking and conversion of ethanol to olefins on SAPO-34 catalyst for the preparation of C4 olefins. Fei Zhang [4] et al. conducted experiments on the reaction performance of methanol, C4 olefins and their co cracking in a fixed bed reactor, explained the problems such as reaction induction period, catalyst stability, and changes in low-carbon olefins yield caused by co cracking, and analyzed the performance of the co cracking catalyst and the application prospect of the co cracking process. Yufeng Pang [5] studied the dehydrogenation performance of the FCC waste catalyst supported catalyst and the supported VOx/Al2O3 catalyst. He prepared the FCC waste catalyst supported catalyst by high-temperature solid phase diffusion method and the VOx/Al2O3 catalyst by impregnation method to prepare C4 olefins. However, it is still insufficient to meet the demand for C4 olefins in China's industry. Ethanol coupling is a commonly used method to prepare C4 olefins, but under some reaction conditions, the conversion of ethanol and the selectivity of C4 olefins are not very ideal. Among them, the reaction temperature, the type of catalyst, and the way of catalyst loading will affect the conversion of ethanol and the selectivity of C4 olefins. Therefore, we studied its ethanol coupling to produce C4 olefins based on the experimental results, analyzed the conversion of ethanol and the selectivity of C4 olefins in terms of reaction temperature, catalyst type and catalyst loading mode, and formulated a reasonable and efficient reaction scheme to maximize the production of C4 olefins, so as to select the best reaction scheme.

2. Data Sources and Model Assumptions

The data in this paper comes from the 2021 National Undergraduate Mathematical Modeling Contest Question B. In order to solve the problem, the research process in this paper is based on the following assumptions: ① The amount of raw materials passing through the unit catalyst in unit time in the chemical reaction process is unchanged; ② When the experiment was stopped at a certain time, the reaction stopped immediately; ③ At the initial stage of the reaction, the catalyst is in full contact with the reactants; ④ The reaction time of each group was the same.

3. Determine the Relationship Between Ethanol Conversion, C4 Olefins Selectivity and Temperature Based on Pearson Correlation Coefficient

3.1. Research Ideas

For different catalyst combinations in Annex 1, the relationship between ethanol conversion, C4 olefins selectivity and temperature was studied respectively. Under different catalyst combinations, the Pearson correlation coefficients between temperature and ethanol conversion, C4 olefins selectivity were calculated using SPSS software, and the results were analyzed. Then the influence of the reaction time of a certain catalyst combination at 350 ℃ on the reaction products and C4 olefins yield was systematically analyzed using MATLAB.

3.2. Research Methods

Pearson correlation coefficient between two variables is defined as the quotient of covariance and standard deviation between two variables [6]:

$$\rho(X,Y)=\frac{\operatorname{cov}(X,Y)}{\sigma_X\sigma_Y}=\frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X\sigma_Y}$$

The above formula defines the overall correlation coefficient, which is usually written in Greek small letters ρ

As a representative symbol. The Pearson correlation coefficient *r* can be obtained by estimating the covariance and standard deviation of the sample

$$r=\frac{\sum_{i=1}^{n}(X_i-\overline{X})(Y_i-\overline{Y})}{\sqrt{\sum_{i=1}^{n}(X_i-\overline{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i-\overline{Y})^2}}$$

Suppose there are two sets of data $X:\{X_1,X_2,\mathtt{B}\ ,X_n\}$ and $Y:\{Y_1,Y_2,\mathtt{B}\ ,Y_n\}$

Sample mean: $\overline{X}=\frac{\sum_{i=1}^{n}X_i}{n}$, $\overline{Y}=\frac{\sum_{i=1}^{n}Y_i}{n}$

Sample covariance [7]:

$$\mathrm{cov}(X,Y)=\frac{\sum_{i=1}^{n}(X_i-\overline{X})(Y_i-\overline{Y})}{n-1}$$

Pearson correlation coefficient of sample: $r_{XY}=\frac{\mathrm{cov}(X,Y)}{S_XS_Y}$

Where, S_X (sigma X) is the standard deviation of the sample, $S_X=\sqrt{\frac{\sum_{i=1}^{n}(X_i-\overline{X})^2}{n-1}}$, Similarly $S_Y=\sqrt{\frac{\sum_{i=1}^{n}(Y_i-\overline{Y})^2}{n-1}}$, The relationship between two data objects can be judged by correlation coefficient.

Through SPSS, correlation analysis was conducted on three groups of data of temperature, ethanol conversionand C4 olefins selectivity under different catalysts, and the phase relationship coefficient table was obtained, as shown in Table 1.

Table 1. Correlation coefficient between temperature and ethanol conversion, C4 olefins selectivity

Catalyst combination	Correlation coefficient between temperature and ethanol conversion	Correlation coefficient between temperature and C4 olefins selectivity
A1	0.965	0.887
A2	0.995	0.914
A3	0.982	0.955
A4	0.998	0.958
A5	0.913	0.978
A6	0.984	0.885
A7	0.999	0.968
A8	0.977	0.992
A9	0.921	0.997
A10	0.923	0.861
A11	0.903	0.989
A12	0.963	0.983
A13	0.936	0.988
A14	0.964	0.959
B1	0.962	0.986
B2	0.929	0.985
B3	0.924	0.945
B4	0.968	0.747
B5	0.964	0.978
B6	0.976	0.959
B7	0.96	0.991

3.3. Result Analysis

According to the solution results in Table 1, under different catalyst combinations, the correlation coefficients between temperature and ethanol conversionand C4 olefins selectivity are greater than 0.8, indicating that temperature is highly correlated with ethanol conversionand C4 olefins selectivity. Based on the data in Annex 1, it can be concluded that the higher the temperature is, the higher the ethanol conversionwill be. However, with the increase of temperature, C4 olefins will occur as a side reaction of reactants, and the temperature also has an impact on the activity of the catalyst. Therefore, C4 olefins selectivity increases first and then decreases with the increase of temperature. At a certain temperature, C4 olefins selectivity reaches the maximum.

According to the test data of a certain catalyst combination at 350 degrees given in Appendix 2, the change rule of selectivity of each product with time can be obtained, as shown in Figure 1. Under the condition of fixed combination of temperature and catalyst, the conversion rate of ethanol gradually decreases to a stable level with the increase of reaction time. After the ethanol conversionstops, the reaction between other products continues.

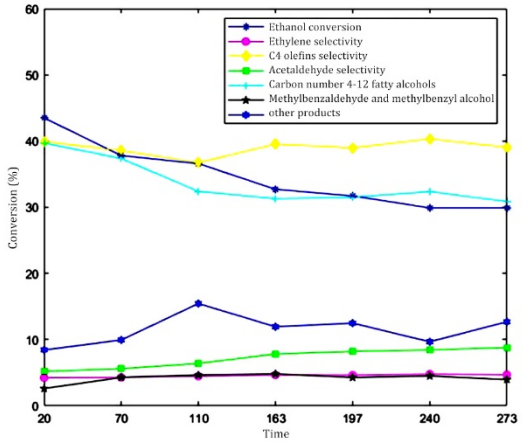

Figure 1. Change rule of product selectivity

At the same time, we calculated by MATLAB that the yield of C4 olefins decreased with the increase of reaction time, as shown in Figure 2. With the increase of reaction time, the reverse reaction in the preparation reaction increases, and the output of the target product decreases. Therefore, the reaction time should be strictly controlled when using ethanol coupling to prepare C4 olefins in industry, so as to maximize the demand of the target product.

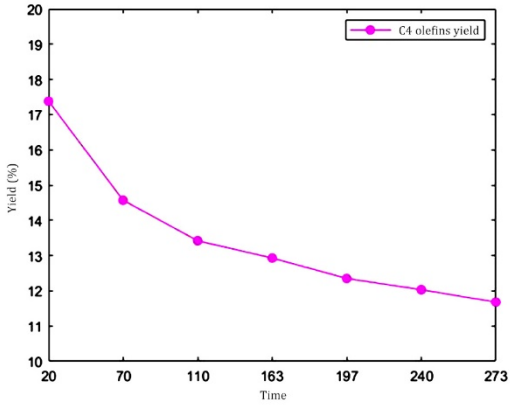

Figure 2. C4 Olefins Yield

4. Determine the Influence of Different Catalyst Combinations and Temperatures Based on Multiple Regression Model

4.1. Research Ideas

The effects of different catalyst combinations and temperatures on ethanol conversionand C4 olefins selectivity were studied. First of all, we conducted a horizontal comparative analysis of different loading methods of the same catalyst to explore the impact of catalyst loading methods on the reaction results. Then a multiple regression model was established to analyze the effects of catalyst and temperature on ethanol conversionand C4 olefins selectivity, respectively.

4.2. Research Methods

4.2.1. Horizontal Comparative Analysis

By drawing temperature ethanol conversionimage and temperature C4 olefins selectivity image for each catalyst combination in Annex 1, and conducting horizontal comparative analysis, if the proportion and dosage of each catalyst are the same when loading in A and B, as shown in Figure 3, the two catalyst combinations have similar ethanol conversionand C4 olefins selectivity, and the loading method has little impact on the reaction [8].

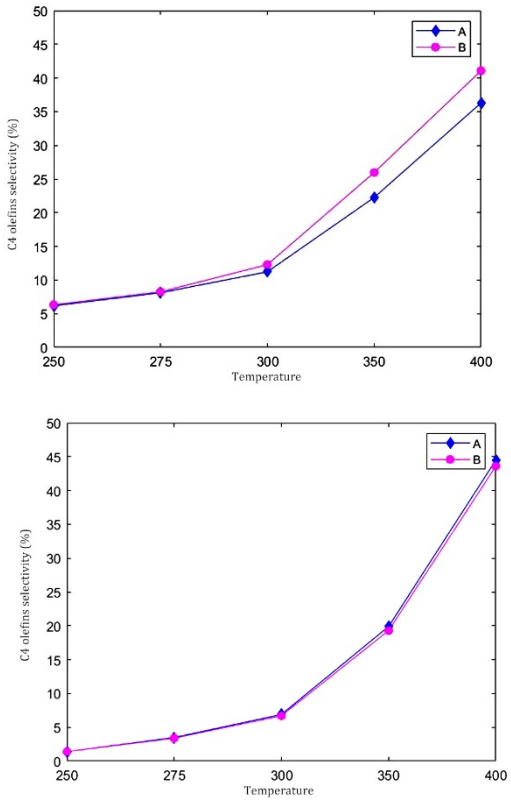

Figure 3. Effect of catalyst loading mode on reaction

Therefore, the catalyst combination data of A and B loading modes were processed uniformly to study the effect of temperature and catalyst combination data on ethanol conversionand C4 olefins selectivity.

4.2.2. Establishment of Multiple Regression Model

In addition to Co/SiO2 HAP in the catalyst classification in Annex 1, Co/SiO2 quartz sand is also used as the catalyst in the A11 combination. However, compared with other groups of Co/SiO2 HAP catalysts, the yield of C4 olefins using Co/SiO2 quartz sand as the catalyst is not high, so we exclude A11 data in the multiple regression analysis. We take ethanol conversionand C4 selectivity as y_1, y_2. Take temperature, amount of each catalyst and ethanol concentration as x_1, x_2, x_3, x_4, x_5. Build a multiple regression model:

$$y_1 = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + C_1$$

$$y_2 = \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 + \gamma_4 x_4 + \gamma_5 x_5 + C_2$$

Calculate the expected value on both sides of the constructed multiple regression equation:

$$E(Y|X_1, X_2, \text{B}\ , X_5) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \text{B}\ + \beta_5 X_5$$

Then, the corresponding estimates of the population parameters are given according to the sample observations [9], and the sample regression equation is obtained:

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \mathrm{B} + \hat{\beta}_5 X_5$$

The least squares estimator is $Q = \sum (Y_i - \hat{Y})^2 = \sum (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_1 - \hat{\beta}_2 X_2 - \mathrm{B} - \hat{\beta}_5 X_5)^2$

Q Calculate partial derivatives of parameters respectively:

$$\begin{cases} \dfrac{\partial Q}{\partial \hat{\beta}_0} = \sum (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_1 - \hat{\beta}_2 X_2 - \mathrm{B} - \hat{\beta}_5 X_5)(-1) = 0 \\ \dfrac{\partial Q}{\partial \hat{\beta}_1} = \sum (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_1 - \hat{\beta}_2 X_2 - \mathrm{B} - \hat{\beta}_5 X_5)(-X_1) = 0 \\ \mathrm{C} \\ \dfrac{\partial Q}{\partial \hat{\beta}_5} = \sum (Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_1 - \hat{\beta}_2 X_2 - \mathrm{B} - \hat{\beta}_5 X_5)(-X_5) = 0 \end{cases}$$

Each parameter of the multiple regression equation can be solved by solving the equations [10].

4.3. Result Analysis

Divide each group of catalysts into four types: Co/SiO2 mass, Co loading, HAP mass and ethanol concentration, and then sort out the data in Annex 1.

Use SPSS to conduct regression analysis on ethanol conversionrate and C4 olefins selectivity, and make ethanol conversion y_1, C4 olefins selectivity is y_2; Temperature, Co/SiO2 mass, Co loading, HAP mass and ethanol concentration are x_1, x_2, x_3, x_4, and x_5 respectively.

First, regress the ethanol conversion, as shown in Figure 4.

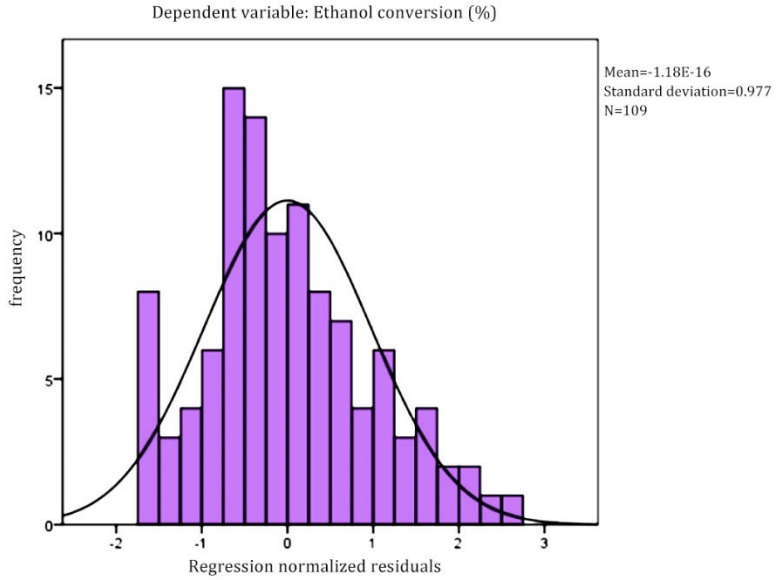

Figure 4. Regression standardized residual of ethanol conversion

Table 2. Ethanol conversioncoefficient

Model	B	Standard error	Standard coefficient	t	Sig.
Constant	-82.934	7.505		-11.051	0
Temperature	0.339	0.02	0.771	17.187	0
Co/SiO2 mass	-0.042	0.1	-0.129	-0.42	0.675
Co loading	-0.345	0.893	-0.018	-0.387	0.7
HAP mass	0.154	0.1	0.475	1.541	0.126
Ethanol concentration	-8.395	2.106	-0.187	-3.987	0

Table 2 shows that at the 95% significance level, the significance level of temperature and ethanol concentration is less than 0.05, indicating that temperature and ethanol concentration have significant effects on ethanol conversionand C4 olefins selectivity. The higher the temperature is, the lower the ethanol concentration is, the higher the ethanol conversionis, and the higher the temperature is, the higher the ethanol concentration is, the greater the C4 olefins selectivity is; However, the significant levels of Co/SiO2 mass, Co loading and HAP mass were all greater than 0.05, and the results were not significant. At the same time, we also know that the catalyst only affects the reaction rate, but does not affect the product output through consulting a large amount of data. Thus, the regression equation can be obtained:

$$y_1 = 0.339x_1 - 8.395x_5 - 82.934$$

Then regress C4 olefins selectivity, as shown in Figure 5.

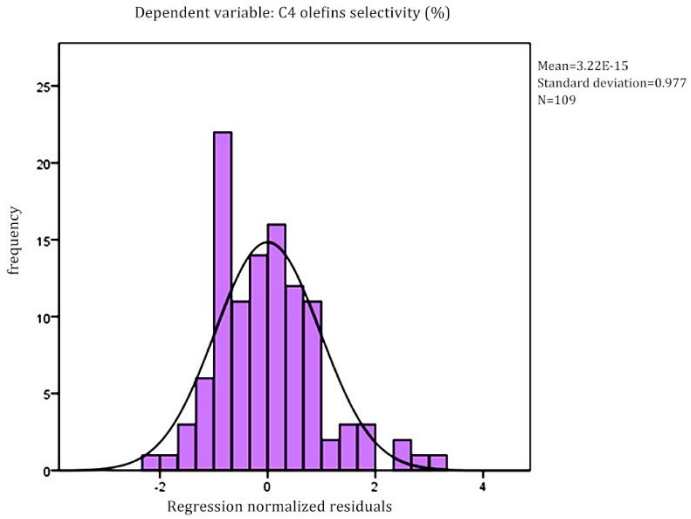

Figure 5. Standardized residual of C4 olefins selective regression

Table 3. C4 olefins selectivity Coefficient

Model	B	Standard error	Standard coefficient	t	Sig.
Constant	-50.003	5.015		-9.97	0
Temperature	0.188	0.013	0.725	14.215	0
Co/SiO2 mass	0.147	0.067	0.773	2.204	0.03
Co loading	-3.061	0.597	-0.268	-5.13	0
HAP mass	-0.063	0.067	-0.332	-0.946	0.346
Ethanol concentration	2.701	1.407	0.102	1.919	0.058

It can be seen from Table 3 that at the 95% significance level, the significance level of temperature, Co/SiO2 mass, Co loading and ethanol concentration is less than 0.05, while the significance level of HAP mass is greater than 0.05, so the regression equation can be obtained:

$$y_2 = 0.188x_1 + 0.147x_2 - 3.061x_3 + 2.701x_5 - 50.003$$

5. Determine the Optimal Catalyst Combination Based on BP Neural Network Model

5.1. Research Ideas

First of all, the catalyst combination and temperature are selected so that the C4 olefins yield is as high as possible under the same experimental conditions, and the BP neural network is used to predict the test results, predict the C4 olefins yield of other temperatures under the catalyst in Annex 1, and then compare and analyze with the given test results to select the most suitable catalyst and temperature combination. Then, the reaction results obtained at different times of the combined reaction of a certain catalyst at 350 °C are compared and analyzed, and the most suitable catalyst and temperature combination at 350 °C are found.

5.2. Research Methods

5.2.1. BP Neural Network Model Establishment

BP neural networks, or forward feedback networks, consist of an input layer, an implicit layer, and an output layer, with each neuron receiving input from the previous layer and outputting to the next layer with no feedback. Nodes are divided into two categories, namely input units and calculation units, each of which can have any input, but only one output. Usually feed-forward networks can be divided into different layers, the input of layer i is only connected to the output of layer i-1, the input and output nodes are connected to the outside world, and the other middle layers are called hidden layers [11]. This is shown in Figure 6.

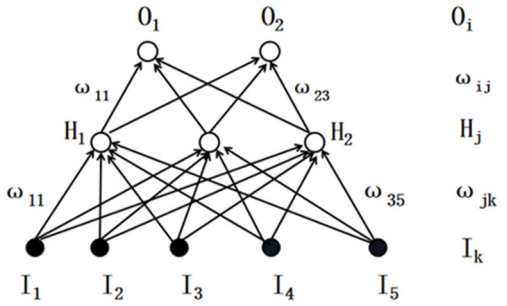

Figure 6. Neural network multivariate Pre-feedback

Because the C4 olefins yield studied is the product of ethanol conversionand C4 olefins selectivity, the C4 olefins yield index is used instead of ethanol conversionand C4 olefins selectivity when the neural network is trained.

In this question, a three-layer BP neural network model with 7 input and 1 output was established with ethylene selectivity, C4 olefins yield, selectivity of butanol, selectivity of carbon number 4-12 fatty alcohol, methylbenzaldehyde and selectivity of methylbenzyl alcohol, and selectivity of other products as the input layer, with the combination of catalyst and temperature as the output layer, and each set of data as the learning sample[12], as shown in Figure 7.

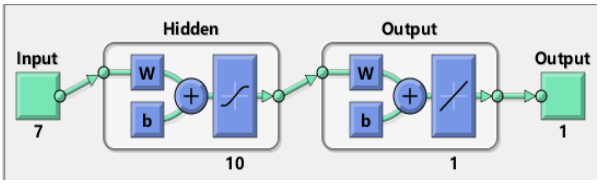

Figure 7. BP neural network model diagram

During the training process, 70% of the samples are taken as the training set, 15% of the samples are used as the test set, and 15% of the samples are used as the validation set, and the Bayesian regularization method is used for sample training [13].

5.2.2. Model Solving

The solution is solved using MATLAB, and the result is shown in Figure 8.

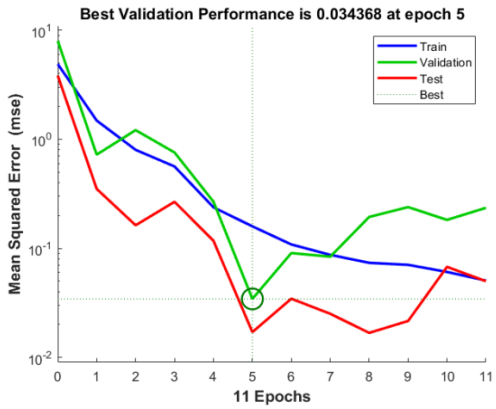

Figure 8. Average squared error plot

The mean squared error is MSE = SSE/n, the minimum value is 0.034368 at the 5th training, and the training continues, because the overfitting effect is affected, so the mean square error rises again. Therefore, the data with the lowest mean squared error is selected as the training result.

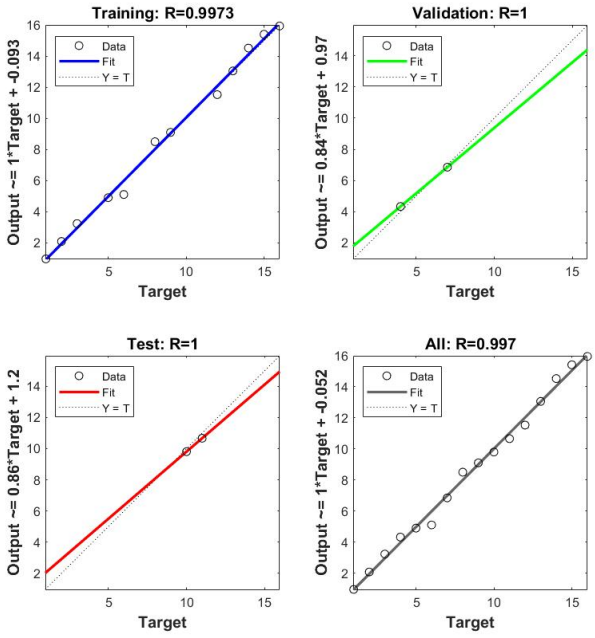

Figure 9. R image

In order to fully compare the C4 olefins yields of different catalyst combinations at various temperatures, we used the sim function to predict that the C4 olefins yields of A1 and A2 catalysts at 400 degrees Celsius were 38.72% and 54.68%, respectively. The highest yield of each catalyst combination at different temperatures was screened out, and the peak yield of C4 olefins of each group of catalysts was plotted, as shown in Figure 10, and the maximum yield of C4 olefins could be obtained at 400 degrees Celsius.

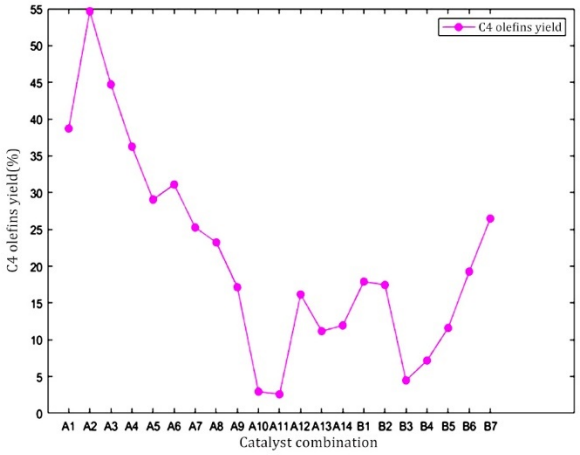

Figure 10. Peak C4 olefins yield of catalysts in each group

5.3. Analysis of Results

In the reaction below 350 degrees, at the beginning of ethanol dehydration to generate ethylene, ethanol conversioncontinues to increase, and ethylene further reacts in the pores of the catalyst, C4 olefins selectivity in addition to the catalyst combination A2, A4, A10, A12, B4 first declined and then rose, the overall state of rising, the remaining catalyst combination of C4 olefins selectivity is increasing, the overall C4 olefins yield is also increasing. Therefore, in the reaction below 350 degrees, the C4 olefins yield showed an increasing trend.

By comparing the magnitude of C4 olefins yield when reacting at 350 degrees under each group of catalysts, it was found that the C4 olefins yield was the highest in the catalyst A2 combination, combined with the increasing trend of C4 olefins yield below 350 degrees, and the catalyst combination A2 was selected to react at 325 degrees when the temperature was lower than 350 degrees, which could make the C4 olefins yield the highest.

5.4. Model Overfitting Test

In the process of training data of BP neural network model, in order to match the training data with the training label, there may be overtraining of the model, resulting in poor generalization ability of the model, which can be used to verify the validity of the model prediction results by retaining some samples and not participating in the training. Using the sim function and the trained model to calculate the predicted value of the retained sample, the comparison chart between the retained sample and the prediction result is plotted, as shown in Figure 11, the predicted data and the original data are highly consistent, and the error is controlled within a reasonable range.

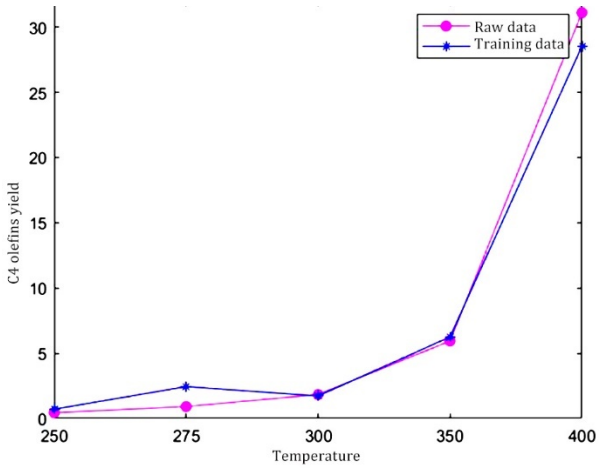

Figure 11. Model test plot

6. Determine the Best Preparation Scheme Based on NetLogo Simulation

6.1. Establishment of Simulation Model

In order to more intuitively simulate the reaction of ethanol coupling to C4 olefins under different experimental combinations, the following simulation model is constructed[14]:

$$C2H5OH \underset{Kd}{\overset{Kc}{<=====>}} C4 + A \xrightarrow{Kr} E + P$$

Wherein C2H5OH represents ethanol C4+ A represents the first stage product, E + P represents the second stage product, the first stage is a reversible reaction, after a certain period of reaction will reach equilibrium, the second stage of the reaction is the reaction to generate by-products, control reaction time can improve C4 olefins yield.

6.2. NetLogo Simulation Results

Using NetLogo software[15], factors other than temperature, catalyst combination, and ethanol concentration are guaranteed in the reaction cell (e.g., pressure, etc.). The reaction cell effect is shown in Figure 12.

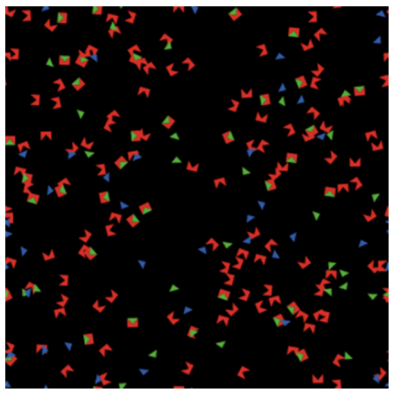

Figure 12. Simulation reaction cell

Multiple simulations were performed to obtain the reaction process under the optimal experimental combination, as shown in Figure 13.

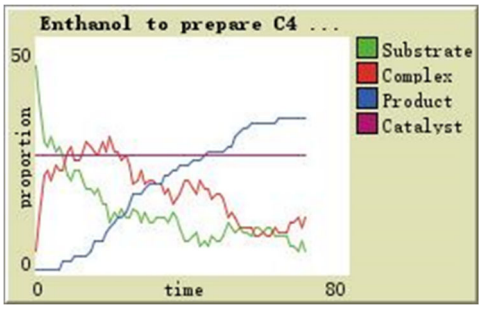

Figure 13. Simulation process diagram

6.3. Analysis of Results

Due to the large interval of experimental temperature selection, it is not possible to fully determine whether the optimal reaction temperature is 400 degrees, so in the first three groups of experiments, we reduce the experimental temperature interval, set the experimental group of 375 degrees and 425 degrees, through NetLogo simulation simulation, it can be seen that the C4 olefins yield of combination two is greater than that of combination one and combination three, so 400 degrees is determined to be the optimal reaction temperature. Then, by changing the Co loading amount and ethanol concentration with high sensitivity to the effect reaction, the optimal reaction temperature for the preparation of C4 olefins and the catalyst combination were investigated by designing combinations four and five, as shown in Table 4.

Table 4. Five-time experimental design table

	Co/SiO2 mass (mg)	Co loading (wt%)	HAP mass (mg)	Ethanol concentration (ml/min)	Temperature (°C)
Combine 1	200	2	200	1.68	375
Combine 2	200	2	200	1.68	400
Combine 3	200	2	200	1.68	425
Combine 4	200	1	200	0.9	400
Combine 5	200	0.5	200	0.9	400

7. Conclusion

In summary, under different catalyst combinations, the higher the temperature, the higher the ethanol conversion, and the C4 olefins selectivity changes with temperature, showing first increase and then decrease, reaching the maximum at a certain temperature. Through regression analysis, it was obtained that the ethanol concentration in the catalyst combination had a significant effect on the ethanol conversion, and the ethanol concentration, Co/SiO2 quality and Co loading amount had a significant effect on the C4 olefins selectivity. By using the BP neural network to synthesize the temperature and catalyst combination, the catalyst combination with the largest C4 olefins yield was A2 group

and the temperature was 400 degrees. At temperatures below 350 degrees, the catalyst combination A2 was chosen at 325 degrees Celsius, with the highest C4 olefins yield. The conclusions were verified by NetLogo simulation.

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