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Study on Preparation of C4 olefins by ethanol coupling based on regression model

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Abstract: *C4 olefin is an important chemical material. The experimental data of C4 olefin preparation by ethanol coupling show that different catalyst combinations and temperatures affect the conversion of ethanol and the selectivity of C4 olefins.It is of great significance and value to explore the process conditions for the preparation of C4 olefins by ethanol catalytic coupling. In this paper, SMO algorithm is used to study that the yield of C4 olefins is the highest when the temperature is 350 ℃; The yield of C4 olefins was the highest when the loading amount of CO was 0.93wt%, the mass of CO / SiO2 was 195.77mg and the temperature was 396 ℃.*

Keywords: *C4 olefin, linear regression model, cluster analysis, correlation analysis*

1. Establishment and solution of model

1.1. Multiple nonlinear regression model

Determine the relationship between the three variables (temperature, ethanol conversion, C4 olefin selectivity, hereinafter referred to as C4).When the sample statistics are used to estimate, the estimated multiple regression equation is:

$$y = \gamma_0 + \gamma_1 x_1 + \gamma_2 x_2 + \gamma_1 x_3^2 + \varepsilon \tag{1}$$

$$Q = \sum(y_i^2 - \acute{y}_i^2) = \sum(y - \gamma_0 - \gamma_1 x_1 - \gamma_2 x_2 - \gamma_1 x_3^2 - \varepsilon) \tag{2}$$

Next, using the least square method, the correlation analysis of the data is made into a matrix diagram, and then the correlation and significance of the data rows are analyzed with the help of SPSS. Finally, the 350℃ thermal analysis diagram is formed with Python.

Model solving:

Use Excel to draw the image and get the factor relationship diagram at 350℃ (as shown in Figure 1).It can be seen from Fig. 1 that the ethanol conversion tends to decrease with the progress of the reaction at 350℃, but the reaction time has little effect on the selectivity of C4 olefins.

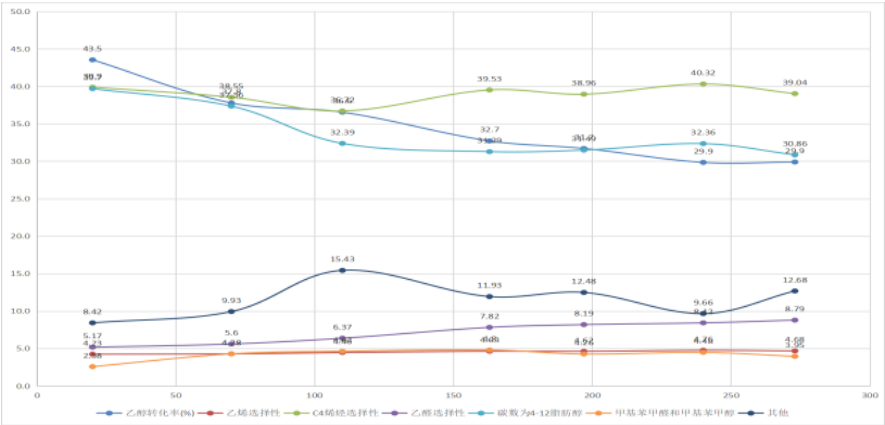

Figure 1: factor relationship at 350 ℃

Use the correl function in Excel to solve the correlation matrix.With the help of MATLAB, the thermal analysis diagram at 350 ℃ is formed for the obtained data .

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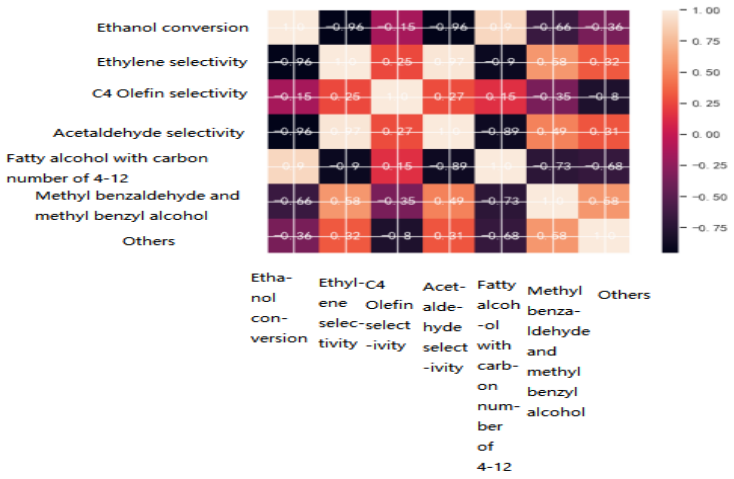

Figure 2: Correlation thermogram analysis at 350 ℃

1.2. Multivariate nonlinear regression model

The catalyst combination is regarded as three variables: CO load, Co / SiO2 mass and ethanol pouring speed. Through Excel data analysis, the ethanol conversion is taken as the dependent variable and the co load, Co / SiO2 mass and ethanol pouring speed are taken as the independent variables to obtain the positive probability diagram (Fig. 2).

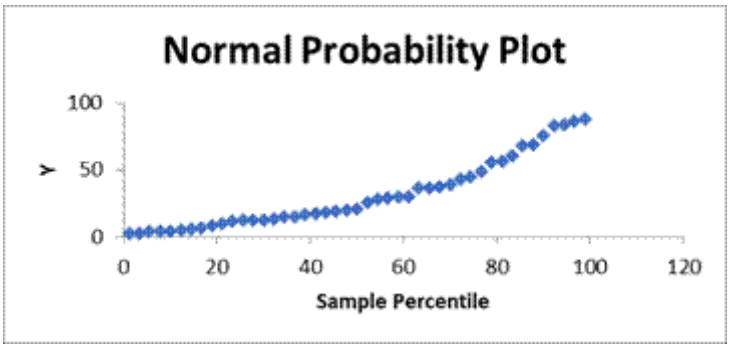

Figure 3: Normal distribution of ethanol conversion with temperature, catalyst

Through data regression analysis, the regression statistical table (Table 2) is obtained.It can be seen from the table that the fitting degree of the data is 86.6%, and the degree of fitting is good.The error is 9.962375827, which is within the allowable range of error.

Table 1: Regression statistics

Regression statistics	
Multiple R	0.930670096
R Square	0.866146827
Adjusted R Square	0.85276151
Standard error	9.962375827
Observed value	45

Taking the catalyst assignment, temperature and catalyst assignment as independent variable x and ethanol conversion as dependent variable y, a multiple nonlinear regression model is established, and the formula is:

$$y = 0.20976x_1 + 0.008089x_2 + 10.91292 \quad (3)$$

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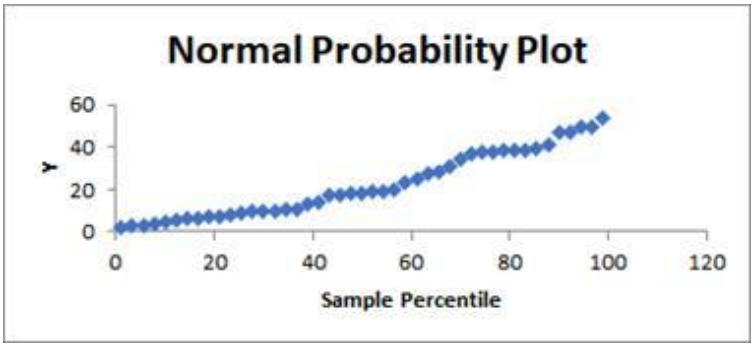

Figure 4: Normal distribution of C4 olefin conversion and catalyst assignment versus temperature

Through the regression model analysis, the regression statistical table is obtained. It can be known that the fitting degree is 52% and the fitting degree is low.

The principle of C4 olefin selectivity is the same as above. The assignment of temperature and catalyst is taken as the independent variable x, and the C4 olefin selectivity is taken as the dependent variable y. it can be known that the equation is:

$$y = -0.28193x_1 + 0.442803x_2 + 12.05079 \quad (4)$$

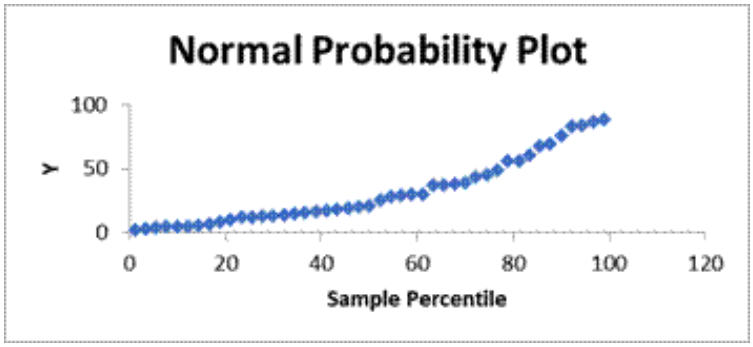

Figure 5: Normal distribution of C4 olefins and assignment catalyst and temperature

1.3. Establishment of statistical regression model

A new multiple ridge regression model integrating radial basis function is established, where Y1 is the conversion of ethanol, Y2 is the selectivity of C4 olefins, and the C4 olefin yield function y:

$$y = \sum_{i=1}^{11}\sum_{j=1}^{11}\gamma_{1i}\gamma_{1j}K(x_i, x_j) \quad (5)$$

In addition, in order to study the situation under the same experimental conditions, it is also necessary to compare the variable with the ethanol conversion Z1 / C4.

The relationship between olefin selectivity Z2 is discussed, and the final goal is:

$$\min y = \sum_{i=1}^{11}\sum_{j=1}^{11}\gamma_{1i}\gamma_{1j}K(x_i, x_j) \quad (6)$$

Solution of statistical regression model:

Establish basic regression statistics to obtain regression statistics (see Table 3).It can be seen from table 3 that the fitting degree is 41.85%, and the fitting degree is low.

Table 2: Regression statistics

Regression statistics	
Multiple R	0.646964
R Square	0.418563
Adjusted R Square	0.405041
Standard error	20.02607
Observed value	45

Using MATLAB to establish three-dimensional graphics, it can be concluded that the C4 olefin yield is the highest at about 396℃ (as shown in figure 6).

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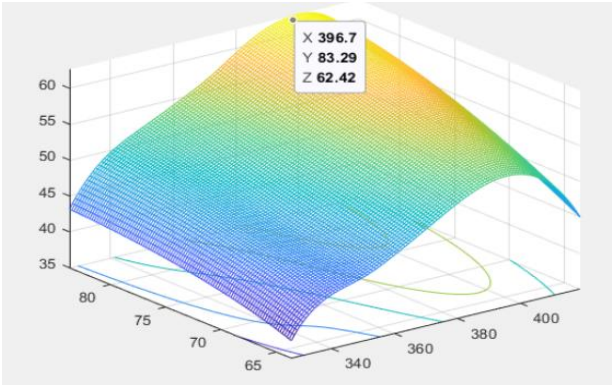

Figure 6: Three-dimensional graphics

According to the ternary ridge model, the highest C4 olefin yield was obtained when the temperature was 396℃; When the temperature is lower than 350℃, the C4 olefin yield is the highest when the temperature is 350℃.

Table 3

Co load (wt%)	Co/SiO2 Quality (mg)	Rate of ethanol intruduction (ml/min)	Temperature	Ethanol conversion	C4 Olefin selectivity	C4 Olefin absorptivity
0.934599	195.7745	0.84213348	396	83.7	62.492415	5231.4514
2.82131	230.4559	1.97456124	350	67.88	43.03577135	2921.23785

2. Advantages and disadvantages of the model

2.1. Advantage

Multiple linear regression analysis is the most basic and simple one in multiple regression analysis.

Using regression model, as long as the model and data are the same, the only result can be calculated through standard statistical methods.

Ridge regression adds a small square deviation factor (in fact, the regular term) to the variable. This square deviation factor introduces a small amount of deviation into the model, but greatly reduces the variance.

2.2. Shortcoming

In the regression analysis, the selected factor and the expression of the factor are only speculation, which affects the diversity of power consumption factors and the immeasurability of some factors.

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