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Research on Effect of catalyst on C4 olefin production

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Abstract: In the process of ethanol coupling to prepare C4 olefins, it is necessary to control variables. How to establish a model for research through mechanism analysis is of great significance to the catalyst conditions for ethanol to prepare C4 olefins and the improvement of product quality. Firstly, this paper uses the regression analysis model to make the change diagram of C4 olefin selectivity of each group of catalysts with the increase of temperature. According to the obtained influencing factors, a multiple regression and function fitting model is established to obtain the weighted numbers of five variables, so as to analyze the effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity.Finally, linprog was used for linear programming to take the yield as the objective function. The maximum value of the objective function was obtained by limiting five factors through constraints. The catalyst combination of 200mg 0.5wt% Co / SiO2 - 200mg HAP ethanol concentration of 0.3ml/min was selected. If there was no temperature limit, the temperature could be increased to 400 degrees.

1. The establishment and solution of the model

1.1 Regression analysis model

According to the established regression analysis model, the selectivity of C4 olefins was solved. For each group of catalysts, the ethanol conversion increased gradually with the increase of temperature.

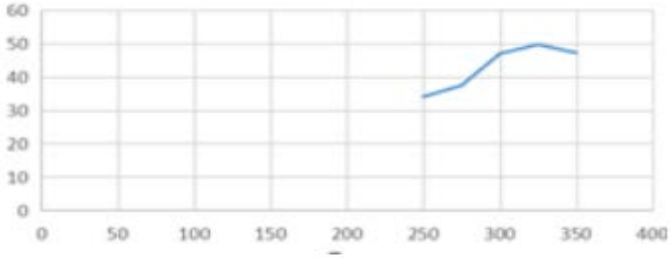

Figure 1: Ethanol conversion of the first group of catalysts

At 350℃, the test results of a given catalyst combination at different times of an experiment will adopt a regression analysis model.Some solutions are as follows:

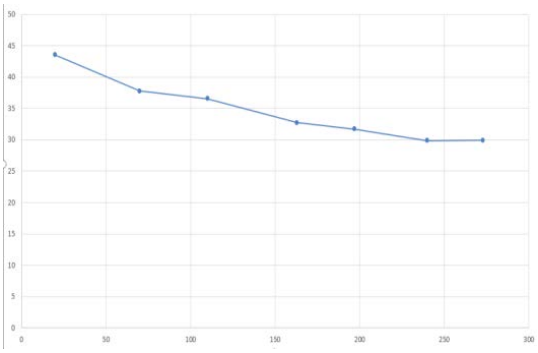

Figure 2: Ethanol conversion (%)

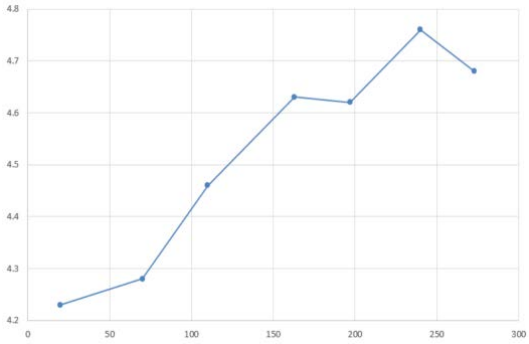

Figure 3: Ethylene selectivity (%)

1.2 Multiple regression and function fitting model

According to the given catalyst combination, five influencing factors are extracted from different combinations, which are Co / SiO2 quality, Co / SiO2 ratio, HAP quality and ethanol concentration. Quartz sand. The ethanol conversion and C4 olefin selectivity were separated according to 250 degrees, 275 degrees, 300 degrees and 350 degrees, and made into excel tables under different catalyst conditions.

Here, taking the fitting of ethanol conversion at 250 degrees as an example, the fitting of other equations is the same. Assume that the multiple linear regression model is:

$$Y_{1,2} = B_0 + B_1X_1 + B_2X_2 + B_3X_3 + B_4X_4 + B_5X_5 + \infty \quad (1)$$

Among them, the random error ∞ includes other factors affecting y. The regress in MATLAB is used for function fitting. The input y is the data of Y in the model (n-dimensional vector, n = 12), X is the data matrix corresponding to the regression coefficient b = (B0, B1, B2, B3, B4, B5) (nx12 matrix, in which the first column is all 1 vector), and alpha is the confidence level a (a = 0.05 by default); Output B is the estimated value B of B, bind is the confidence interval of B, R is the residual vector, rint is the confidence interval of R, stats is the test statistic of the regression model, there are three values, the first is the determination coefficient R2 of the regression equation (R is the correlation coefficient), the second is the value of F statistic, and the third is the probability value p corresponding to the value of F statistic. The following figure shows the values solved by MATLAB.

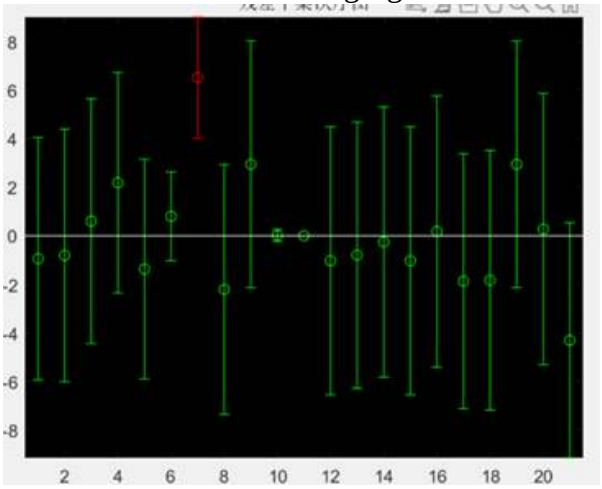

Figure 4: Sequence of residual cases

Model validation:

Correlation R is usually the correlation coefficient.If the absolute value of R is in the range of 0.8-1, the relationship between regression variables can be determined. In this example, R2 = 0.7379.The absolute value of R is 0.8590, which indicates a strong correlation.

Finally, the weighted values of five influencing factors can be obtained by tabulating the coefficients in all equations, with ethanol conversion on the left and C4 olefin selectivity on the right

Table 1: Weighted values of influencing factors

	250℃	275℃	300℃	350℃	250℃	275℃	300℃	350℃
Constant term	12.9371	16.3869	17.2739	25.1992	-2.1882	0.3366	4.8402	16.89
X1	-0.0077	-0.0024	-0.0052	-0.0132	0.060	0.0020	0.0054	0.0056
X2	20.3962	0.5673	0.7110	1.8604	2.8513	-2.2145	-3.7660	-6.1171
X3	0.0116	0.0352	0.0994	0.1848	0.0617	0.0627	0.0768	0.0984
X4	-7.7974	8.2300	8.6930	-9.3631	4.2119	3.3900	3.0609	2.8963
X5	-0.0184	-0.0279	-0.0169	-0.0274	-0.0248	-0.0324	-0.0519	-0.1286

1.3 linear programming model

Firstly, the catalyst combination with the highest yield is obtained by using the data of 250 degrees, 275 degrees, 300 degrees and 350 degrees, and then the results are used to analyze the situation greater than 350 degrees.According to the calculated C4 olefin yields of different catalysts at 250℃, 275℃, 300℃ and 350℃, the data are sorted out, and the linear programming is carried out by using Matlab's linprog to obtain the catalyst combination that can achieve the highest yield at four temperatures. The following table is the calculated results

Table 2: Catalyst combinations with the highest yield at different temperatures

	250degree	275degree	300degree	350Degree
X1	10	200	200	200
X2	5	0.5	0.5	0.5
X3	200	200	200	200
X4	0.3	0.3	0.3	0.3
X5	0	90	90	0
yield	76.3519	196.5599	579.2432	1878.1849

By analyzing the table, first look at the catalyst combination at different temperatures. It can be seen that X1 and X3 are 1:1 except 250 degrees. Therefore, when the ratio of these two is 1:1, the yield is the largest.At the same time, X2 is better taken as 0.5 and X4 is taken as 0.3. For quartz sand x4, because there is only one set of data given, the analysis results are of little significance, and this condition will not be considered first.Looking at the temperature again, it is found that with the increase of temperature, although the catalyst combination is different, the yield has been rising, and the rising range gradually increases. Therefore, when the temperature is greater than 350℃, the yield will continue to rise.Finally, it is concluded that if the temperature is below 350℃, the catalyst combination of 200mg 0.5wt% Co / SiO2 - 200mg HAP ethanol concentration of 0.3ml/min can be selected. If there is no temperature limit, the temperature can be increased to 400℃.

2. Evaluation of the model

(1) The regression analysis model is used to accurately produce the relationship between ethanol conversion and temperature, the relationship between C4 olefin selectivity and temperature, and the relationship between product content of a given catalyst combination at 350℃ at different times of an experiment. Although the change of the relationship can be listed in a relatively simple way to avoid the possibility of falling into a local optimal solution, However, it is difficult to analyze the more complex relationship between them more accurately.Although it can accurately express the changes in the relationship between the two, it is too complex to use other software to analyze the composition

(2) The established multiple function regression model uses MATLAB to solve the relationship between the effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity, which can more accurately judge the relationship between them, but it can not be solved quickly, and the process is numerous, complex and error prone.

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