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Study on Preparation Process of Ethanol Coupled Olefins Based on Multi-objective Programming

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Abstract: *Ethanol molecules can be prepared by biomass fermentation, with a wide range of sources, green and clean. Using ethanol as a platform to produce high value-added and C4 olefins has great application prospects and economic benefits have attracted wide attention at home and abroad. In this paper, considering the combination of each group of catalysts, the relationship between ethanol conversions, that is, the selectivity of C4 olefins was explored, and the regression model was used to establish it. The data in the table were screened and solved by MATLAB program, and the relevant data were obtained. Then, considering the correlation between different catalyst combinations and two dependent variables, three indexes affecting the catalyst are obtained, and then the temperature is combined. Four independent variables and two dependent variables were analyzed. Multiple regression model, least square method and MATLAB method were used for regression operation. Finally, on the basis of the multiple regression established, the stepwise regression analysis is used to select the appropriate decision variables and constraints for multivariate programming, and the MATLAB algorithm is used to solve the problem. Finally, it is concluded that the yield of C4 olefin is 44.73% when the loading ratio of Co load is 1wt%, the loading ratio of HAP is 200mg, the concentration of ethanol is 0.9ml/min, and the temperature is 400C. Under the constraint condition of the second half of 350C and adding the constraint conditions on the basis of the original, it is concluded that the highest yield of 26.54% is obtained when the loading ratio of Co load 2wt% HAP to HAP is 200mg, the concentration of ethanol is 1.68ml/min, and the temperature is 350C.*

Keywords: *Linear programming, Control variable, Multiple regression*

1. Introduction

The production of chemical products and medicine requires the participation of C4 olefin, and ethanol is the raw material for the preparation of C4 olefin. Ethanol molecules can be prepared by biomass fermentation, from a wide range of sources, green and clean[1], using it as a platform for the production of high value-added and C4 olefin has great prospects and economic benefits has been widely concerned at home and abroad.

2. Regression process analysis

For the combination of 21 kinds of catalysts, the regression analysis relationship was selected to better explain the degree of fitting between them. Statistical regression of fractional correlation coefficients was used:

$$\text{s}\, R^2 = \frac{SSR}{SST} - \frac{\sum_1^n \left(\hat{y}_i - \bar{y}\right)^2}{\sum_1^n \left(y_i - \bar{y}\right)^2} \tag{1}$$

As a result, the correlation coefficients under the degree of linear and nonlinear fitting can be obtained [2].

Under the condition of linear fitting, the correlation coefficient of some data R^2 has low correlation, so it is not persuasive. However, under the condition of nonlinear fitting, the correlation coefficients are close to 1, indicating that nonlinear fitting is more conducive to the establishment of the relationship between the two.

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Table 1: The relationship between the temperature of each catalyst combination and ethanol conversion (Part)

Catalyst group	Correlation coefficient under the degree of linear fitting	Correlation coefficient under nonlinear fitting degree
A1	0.9322	0.9797
A2	0.9900	0.9911
A3	0.9643	0.9663
A4	0.9950	0.9959
A5	0.8734	0.9940
B1	0.9256	0.9989
B2	0.8635	0.9913
B3	0.7924	0.9915
B4	0.8087	0.9870
B5	0.8325	0.9914

3. Model of ethanol conversion and C4 olefin selectivity under different parameters

Multivariate regression equation was introduced, and the least square method was combined with MATLAB algorithm for analysis [3] [4]:

$$\begin{aligned} y_1 &= \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_4 x_4 + z_1 \\ y_2 &= \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + z_2 \end{aligned} \tag{2}$$

The establishment process of the formula:

$$\begin{cases} \sum y = nz + \alpha_1 \sum x_1 + \alpha_2 \sum x_2 + \alpha_3 \sum x_3 + \alpha_4 \sum x_4 \\ \sum x_1 y = z \sum x_1 + \alpha_1 \sum x_1^2 + \alpha_2 \sum x_1 x_2 \\ \sum x_2 y = z \sum x_2 + \alpha_1 \sum x_1 x_2 + \alpha_2 \sum x_2^2 \end{cases} \\ \begin{cases} \sum x_3 y = z \sum x_3 + \alpha_3 \sum x_3^2 + \alpha_4 \sum x_3 x_4 \\ \sum x_4 y = z \sum x_4 + \alpha_3 \sum x_3 x_4 + \alpha_4 \sum x_4^2 \end{cases} \tag{3}$$

Finishing the influence of various catalyst combinations and parameters at temperature:

Table 2: y1 Relation between parameters

Parameter	Coefficient
α_1	0.14
α_2	0.15
α_3	-8.75
α_4	0.34
z_1	-82.59

The regression equation:

$$y_1 = 0.14x_1 + 0.15x_2 - 8.75x_3 + 0.34x_4 - 82.59 \tag{4}$$

Table 3: y2 Relation between parameters

Parameter	Coefficient
β_1	-3.20
β_2	-0.086
β_3	2.82
β_4	0.19
z_2	-50.07

The regression equation:

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$$y_2 = -3.20x_1 - 0.086x_2 + 2.82x_3 + 0.19x_4 - 50.07 \tag{5}$$

According to the regression equation, temperature has the greatest influence on ethanol conversion [5], Co loading has the least influence on ethanol conversion, Co loading has the greatest influence on C4 olefin, and Co/SiO2 / HAP charging ratio has the least influence on C4 olefin selectivity.

4. Optimal combination and Optimization Model of temperature

The yield of C4 olefins = conversion of ethanol × selectivity of C4 olefins. The variables were temperature, Co loading capacity, Co/SiO2 and HAP loading ratio. The amount of Co, the ratio of Co/SiO2 to HAP, and ethanol affect the effect of catalyst

$$\begin{aligned} z_3 = y_1 \times y_2 = &\left(0.14x_1 + 0.15x_2 - 8.75x_3 + 0.34x_4 - 82.59\right)\times \\ &\left(-3.20x_1 - 0.086x_2 + 2.82x_3 + 0.19x_4 - 50.07\right) \end{aligned} \tag{6}$$

Decision variables:

$$\begin{cases} x_1\{0.5,1,2,5\}, x_2\{10,25,50,75,100,200\} \\ x_3\{0.3,0.9,1.68,2.1\}, x_4\{250,275,300,325,350,400\} \\ x_1x_2x_3x_4 > 0 \end{cases} \tag{7}$$

Constraints:

$$\begin{cases} x_1 + x_2 \le 205, x_3 + x_4 \le 402.1 \\ x_1 + x_3 \ge 7.1, x_2 + x_4 \ge 260 \end{cases} \tag{8}$$

Under the same experimental conditions, the temperature is within the desirable range, planning and solving [6]. MATLAB was used to solve the optimal solution, that is, the maximum yield of C4 olefin.

Table 4: Optimal planning data

x_1	1wt%
x_2	200mg
x_3	0.9ml/min
x_4	400ºC
z_3	44.73%

Multiple regression analysis and stepwise analysis is a reasonable scientific study of data. However, for the preparation of C4 olefin by ethanol coupling, the dependent variable is restricted by a variety of factors, and this analysis method is established to carry out reasonable operation, and the results can be tested by R2 test, T test and F test. Establish the significance of regression curve, and then get reasonable prediction results.

Then set 350 degrees as the limiting condition, carried out the temperature limit below 350℃, under this limit, continue to use stepwise regression analysis.

$$s.t.\{x_4 <= 350\} \tag{9}$$

Table 5: Optimally plan data under temperature constraint

x_1	2wt%
x_2	200mg
x_3	1.68ml/min
x_4	350ºC
z_3	26.54%

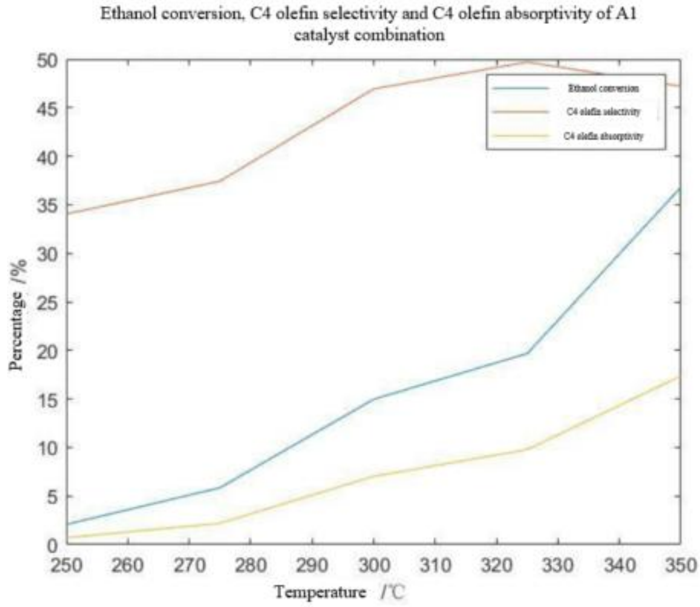

Figure 1: C4 olefin yield varies with temperature

For the test of optimization class, the stability and correctness of the model should be judged. When the temperature is limited, the coefficients of the variables α and β establish a range of values. The results of subsequent operational tests showed little change in the range. $y = ax + b, y = ax^2 + bx + c$. These fitted equations are still stable within the range after further test and analysis, so the rationality of the test is good for the above two models and can be used as regression analysis.

5. Conclusion

First of all, this paper explores the relationship between ethanol conversions, that is, the selectivity of C4 olefins, and establishes it by using the regression model. It is found that there is no obvious linear correlation between ethanol conversion and C4 olefin selectivity of A11 and B3 catalysts, but there is an obvious non-linear correlation between ethanol conversion and C4 olefin selectivity of almost all catalyst combinations and temperature. Then, considering the correlation between different catalyst combinations and two dependent variables, the analysis of four independent variables and two dependent variables was carried out. Multiple regression model, least square method and MATLAB method were used for regression operation. Finally, on the basis of multiple regression, the stepwise regression analysis is used to select the appropriate decision variables and constraints for multivariate programming, and the MATLAB algorithm is used to solve the problem. Finally, it is concluded that the yield of C4 olefin is 44.73% when the loading ratio of Co load is 1wt%, the loading ratio of HAP is 200mg, the concentration of ethanol is 0.9ml/min, and the temperature is 400C.

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