

Research on Preparation of C4 Olefin Process Based on Multiple Linear Regression

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Abstract: Ethanol has a wide range of molecular sources, outstanding functions and environmental protection. The preparation of C4 olefins by ethanol molecular coupling has a large-scale application direction and economic benefits of sustainable development. In this paper, a corresponding model is established to analyze the catalyst combination factors that affect the preparation of C4 olefins by ethanol coupling. Firstly, all scatter plots between temperature and ethanol conversion rate and scatter plots between temperature and C4 olefin selectivity are made, and nonlinear fitting is carried out. Secondly, the relationship between different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity was analyzed, and the fitting equations of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity were obtained by multiple linear regression, thus reflecting the relationship between ethanol conversion, C4 olefin selectivity and each catalyst combination.

1. Introduction

With the rapid improvement of material living standards, the number of household vehicles is increasing rapidly, and the socio-economic level is also developing rapidly, resulting in the shortage of global fossil energy output. Therefore, it is an urgent task to find an alternative renewable and developable new energy source. At the same time, the ecological environment has also been damaged to a certain extent, leading to the frequent occurrence of rare diseases of human beings around the world, so high-quality medical drugs become essential. In this urgent situation, in order to solve this kind of problems with high efficiency and low cost, [1] It is of great significance and value to explore the technological conditions of preparing C4 olefins by catalytic coupling of ethanol. [2]

2. Analysis of Temperature Influence Based on Nonlinear Fitting

At discrete points $[(x_1, y_1), (x_2, y_2), (x_3, y_3) \dots (x_m, y_m)]$, get the resolution function $y=f(x)$, and let $f(x)$ approach the given value of y_j at the original discrete point x_j as much as possible. This process is called curve fitting. According to the data set, in solving practical problems, we can draw a scatter diagram through the known data set, and analyze and design the curve types that need to be fitted through the data set and scatter diagram. According to MATLAB, the scatter diagram of ethanol conversion rate, C4 olefin selectivity and temperature is obtained.

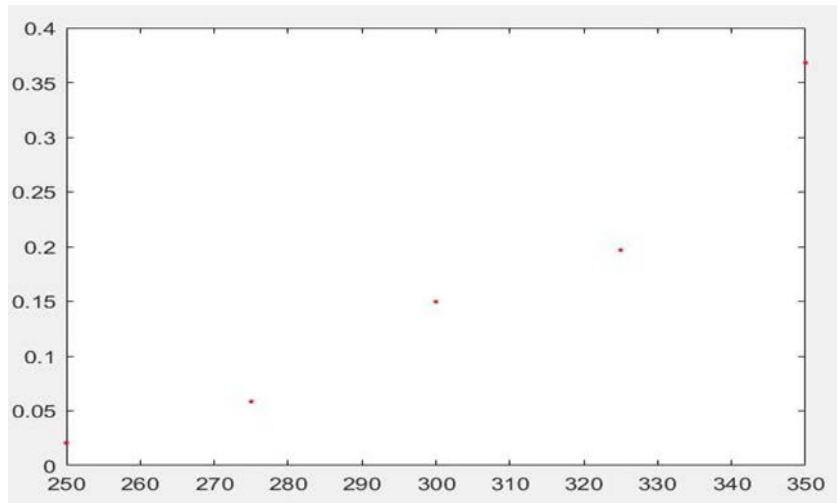


Figure 1: Scatter diagram between temperature and ethanol conversion rate

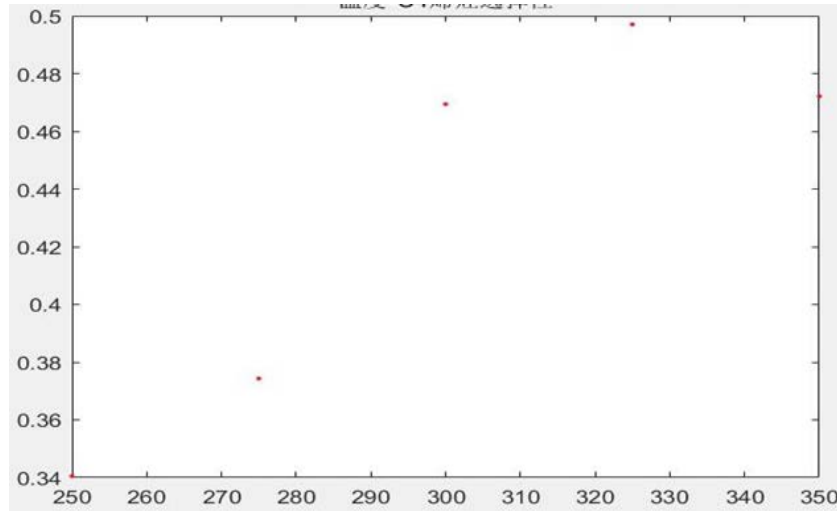


Figure 2: Scatter diagram between temperature and C4 olefin selectivity

When the sum of squares of the deviation between the function value of the function $f(x,y)$ at the point x_j ($j = 1,2,3,4,5$) and the observed data reaches the minimum, it is the function we are looking for. The following conditions must be met:

$$\min g(x) = \sum_{j=1}^5 (f(x_j, y') - y_j)^2$$

Let the determinable coefficient R^2 be

$$R^2 = 1 - \frac{\sum_{j=1}^5 (y_j - y_i')^2}{\sum_{j=1}^5 (y_j - \bar{y})^2}$$

$$\bar{y} = \frac{1}{n} \sum_{j=1}^5 y_j$$

When R^2 is closer to 1, the better the fitting effect, the closer it is to nonlinear fitting.

The following figure shows the image obtained by the third-order nonlinear fitting function with high fitting degree in MATLAB.

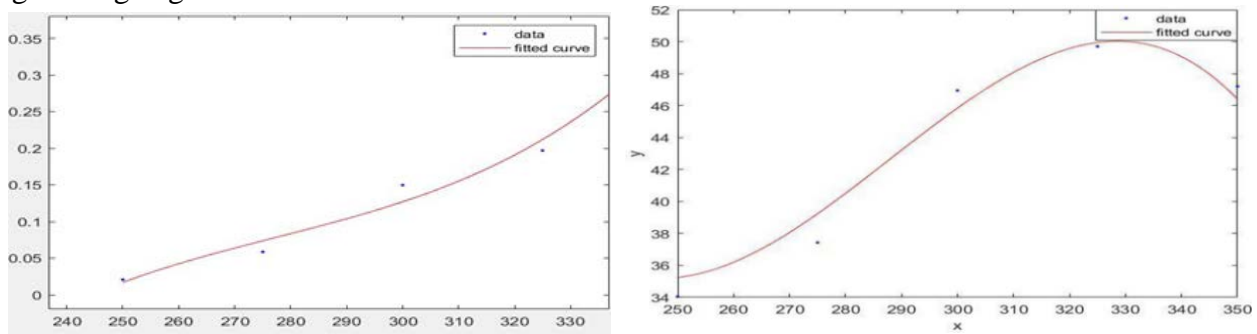


Figure 3: Nonlinear fitting image

3. Process Model of Multiple Linear Regression

Multiple regression analysis is a regression analysis method to study the relationship between multiple variables, to determine the possible forms of the number of variables, and to use mathematical models to express as follows [3]:

$$Y = \beta_0 + \sum_{i=1}^k \beta_i X_i + \varepsilon$$

To establish the model, we should test the fitting degree of the model. The significance test of the regression equation is to test whether the linear relationship of the variables of the sample regression equation is significant, that is, whether at least one of the multiple regression coefficients in the overall regression equation can be inferred from the sample is not equal to 0, which mainly shows the significance of the sample regression equation R^2 .

According to the correlation analysis, the ethanol conversion rate has a great correlation with the concentration, Co dosage, temperature, HAP dosage and SiO₂ dosage in each catalyst, and the C₄ olefin selectivity has a great correlation with the temperature, HAP dosage and SiO₂ dosage in each catalyst. The multiple linear regression is analyzed by SPSS, and the fitting equation of the linear relationship is obtained.

According to the size of R^2 , the fitting degree of multiple linear regression equation can be judged, and the error between R^2 value and standard estimation can be obtained by observing the model back three times, with $R^2=0.796$, which shows that the equation fits well. Finally, the linear regression equation of ethanol conversion rate and catalyst combination is as follows:

$$Y1 = 0.109x1 - 8.654x2 + 0.339x3 - 82.612$$

x_1 , x_2 and x_3 represent the dosage, concentration and temperature of HAP respectively.

Similarly, according to the size of R^2 , we can judge the fit of multiple linear regression equation, and observe that the model retreats three times to get the error between the value of R^2 and the standard estimate, $R^2=0.711$, which shows that the equation has a high fit. Finally, the linear regression equation of C₄ olefin selectivity and catalyst combination is as follows:

$$Y2 = -1.786x1 - 0.186x2 + 0.106x3 - 49.528$$

x_1 , x_2 and x_3 represent the amount of Co, temperature and SiO₂, respectively.

The above two equations can represent the relationship between different catalyst combinations and temperatures on ethanol conversion and C₄ olefin selectivity.

4. Conclusion

In this paper, correlation analysis and multiple linear regression are used to analyze the relationship between ethanol conversion rate, C4 olefin selectivity and catalyst combination, and the relationship between them is established effectively. It provides some guidance for preparing C4 olefins by ethanol catalytic coupling with high efficiency and low cost.

References

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