Journal of Materials, Processing and Design (2021) 5: 50-53
Clausius Scientific Press, Canada
DOI: 10.23977/jmpd.2021.050110
ISSN 2516-0923

Research based on optimization model of C4 olefins preparation

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Keywords: Linear relationship, Multivariate function, Optimization design

Abstract: In this paper,the data given by the topic are studied,and the model is established and optimized.Firstly,the function relationship was established.The least square method was used to calculate the coefficient of each variable,so as to obtain the linear relationship between the data,and the correlation coefficient was obtained through the linear relationship[1].Then the temperature and different ingredients have a great influence on the conversion of ethanol and C4 olefin selectivity.Establish multivariate function,by comparing the size of correlation coefficient,by controlling the single variable method,for different combinations of groups to achieve the effect of a single variable,these data are converted into line graph,and then find out the optimal catalyst combination and temperature in each group.

1. Background

C4 olefins are widely used in chemical and medical fields, and ethanol is the raw material for the production and preparation of C4 olefins.Traditional production methods all use fossil energy as raw materials, but with the shortage of fossil energy output and the aggravation of environmental impact, the supply of energy gradually tends to diversify, the development of new clean energy is more and more urgent. It is of great significance and value to study the technological conditions of preparing C4 olefin by ethanol catalytic coupling through the design of catalyst combination.

2. Model Establishment

2.1 Establishment of regression equation

According to the problem analysis, the following model is established: The linear regression model of random variable Y and independent variable X is:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p \tag{1}$$

When there are n groups of observation data, the regression model can be expressed in matrix form:

$$y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}, x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} \end{bmatrix} \tag{2}$$

According to regression analysis theory, for an excellent fitting equation[2], the sum of residuals should be as small as possible. When the residual is smaller, the fitting value is closer to the observed value, and the observation points are highly clustered around the fitting line, and the tightness degree is higher.In other words, the fitting equation $y = \widehat{\beta_0} + \sum_{i=1}^{6} \widehat{\beta_1} x_i$ explain y ability is stronger.

$SST = \sum_{i=1}^{n} (y_i - \widehat{y_i})^2$, Where, SST is the sum of squares of the total variation of y_i, and its degree of freedom is $df_T = n - 1$.

$SSR = \sum_{i=1}^{n} (\widehat{y_i} - \bar{y}_i)^2$, The SSR for fitting line $y = \widehat{\beta_0} + \sum_{i=1}^{6} \widehat{\beta_1} x_i$ used to interpret the variation of sum of squares, its degree of freedom for $df_R = 1$.

$SSE = \sum_{i=1}^{n} (y_i - \widehat{y_i})^2$, Where SSE is the sum of squares of residuals, and its degree of freedom is $df_E = n - 2$.

$$\mathbf{SST} = \mathbf{SSR} + \mathbf{SSE} \quad df_T = df_R + df_E \tag{3}$$

It can be seen from the above formula that the variation of y is caused by the following two reasons: First, the different values of x lead to systematic variation of Y.The other reason is the influence of other factors besides x, and we know that SST is a fixed value[3]. Therefore, it can be explained that the larger the SSR variation is, the smaller the SSE residual is. This decomposition can explain the good degree of the fitting equation from two aspects simultaneously:

(1) The larger the SSR is, the larger the proportion of y_i variation explained by regression equation, and the better the regression equation explained the original data;

(2) The smaller SSE is, the closer the observed value y_i is around the regression line, and the better the regression equation can fit the original data.

Therefore, define a measure to describe the degree of fit between the regression equation and the original data.Assume that the minimum of $\varepsilon = y - X\hat{\beta}$ can be found according to the extreme calculus principle:

$$\frac{\partial Q}{\partial \hat{\beta}} = \frac{\partial (y - X\hat{\beta})(y - X\hat{\beta})}{\partial \hat{\beta}} = 0 \tag{4}$$

To fit the effect, the temperature needs to be dimensionless:

$$\mathrm{T} = \frac{\mathrm{x} - \bar{\mathrm{x}}}{\sigma} \tag{5}$$

After MATLAB calculation, the regression equation of ethanol conversion rate without quartz sand was obtained:

$$y_{11} = 38.5231 + 1.4008x_1 + 1.9013x_3 - 13.8991x_4 + 17.2715x_5 \tag{6}$$

The regression equation of ethanol conversion with quartz sand is as follows:

$$y_{12} = 40.0284 - 18.3774x_2 + 1.7468x_3 - 13.5392x_4 + 17.2716x_5 \tag{7}$$

The regression equation of C4 olefins selectivity without quartz sand is as follows:

$$y_{21} = 14.0164 + 7.2114x_1 - 1.7653x_3 - 1.4282x_4 + 9.3696x_5 \tag{8}$$

The regression equation of C4 olefins selectivity with quartz sand is as follows:

$$y_{22} = 21.3497 - 26.2211x_2 - 1.9456x_3 - 1.0085x_4 + 9.3696x_5 \tag{9}$$

2.2 Establishment of multivariate functions

Firstly, quantitative analysis is carried out:

(1) Assume that z_1 is the conversion rate of ethanol and z_1 is the selectivity of C4 olefin; x is the catalyst and y is the temperature.

(2) a_1 is the mass ratio of Co/SiO2 to HAP,a_2 is quartz sand,a_3 is Co load,a_4 is the amount of ethanol concentration poured in a minute,and a_5 is the temperature.

The function expression of random variable y and independent variable x is:

$$z = f(x, y) \quad (10)$$

$$x = f(a_1, a_{2,} a_3, a_4, a) \quad (11)$$

The larger the regression coefficient is, the greater the influence of x variable on y variable is.The positive regression coefficient means that y increases with the increase of x, and the negative regression coefficient means that y decreases with the increase of x.

When P value is lower than 0.01, it is very significant.P value between 0.01 and 0.05 is significant; P > 0.05 is not significant.

2.3 Results of the model

For the ethanol conversion rate without quartz sand,the amount of ethanol concentration and temperature in one minute have the greatest influence on the ethanol conversion rate.For the ethanol conversion with quartz sand,the quality and temperature of quartz sand have the greatest influence on the ethanol conversion.For the selectivity of C4 olefin without quartz sand,Co/SiO2 and HAP ratio X1 and temperature have the greatest influence on the selectivity of C4 olefin.For C4 olefins selectivity with quartz sand,quartz sand has the greatest influence on C4 olefins selectivity.

3. Analysis of model results

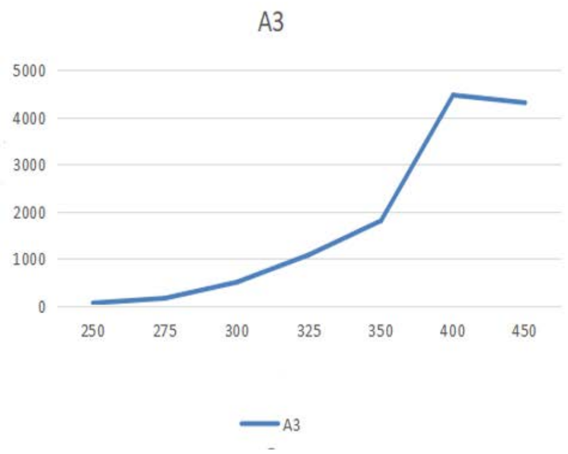

Figure 1: Reaction temperature

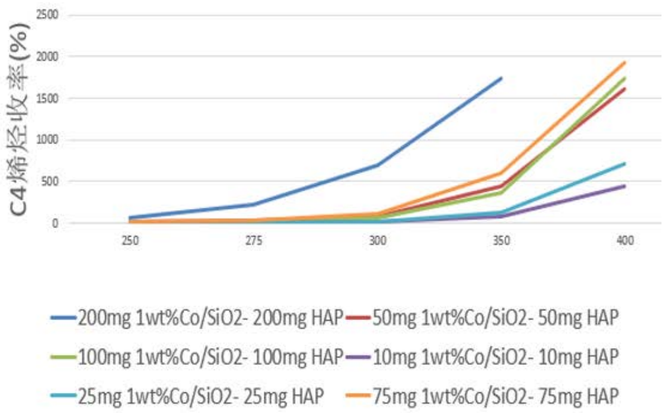

Figure 2: Loading ratio

Reaction temperature: According to the data, when the reaction temperature is 400°IC, the yield of C4 olefin, the conversion of ethanol and the selectivity of C4 olefin both reach relatively high values. Due to the limited data, as shown in Figure 1,400°C is the suitable temperature for catalytic reaction only based on the data of A3 group catalyst combination and other catalyst combination.

Loading ratio:Under the condition of 1wt% Co loading,the mass ratio of Co/SiO2 and HAP is 10mg:10mg,the mass ratio of Co/SiO2 and HAP is 25mg:25mg, the mass ratio of Co/SiO2 and HAP is 50mg: 50mg,the mass ratio of Co/SiO2 and HAP is 75mg: The data of 75mg,Co/SiO2 and HAP mass ratio of 100mg: 100mg and Co/SiO2 and HAP mass ratio of 200mg: 200mg were analyzed. According to Figure 2, when the reaction temperature was 400°C, the mass ratio of Co/SiO2 and HAP was 75mg: The yield of C4 olefins was the highest at 75mg. The maximum yield of C4 olefins was obtained when the reaction temperature was 350°C and the Co/SiO2 / HAP mass ratio was 200mg: 200mg.

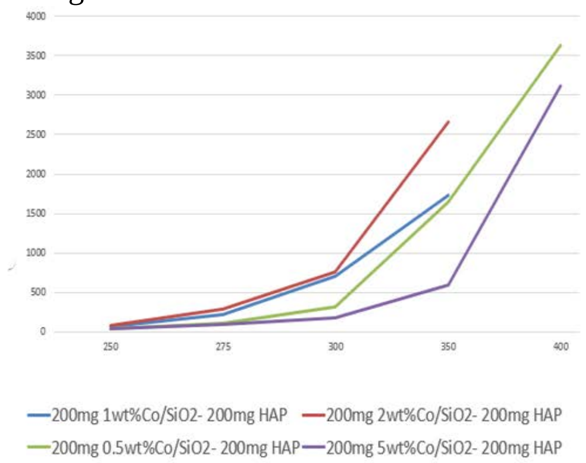

Figure 3: Co load

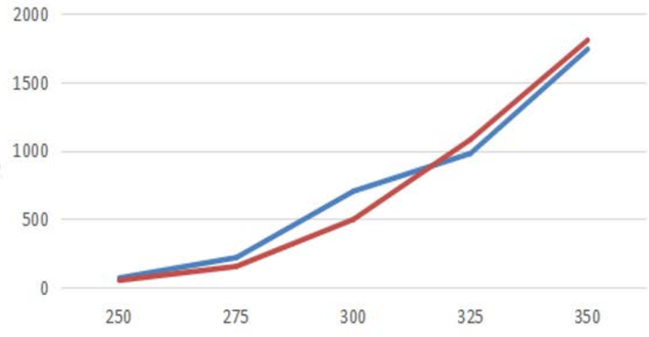

Figure 4: Different ethanol concentration per minute

Co load: According to the conclusion and data, the mass ratio of Co/SiO2 to HAP is 200mg: Under the condition of 200mg, the data of Co loading of 0.5wt%, Co loading of 1wt%, Co loading of 2wt% and Co loading of 5wt% were analyzed. According to Figure 3, when the reaction temperature was 400° C, the yield of C4 olefins was the highest under the condition of Co loading of 0.5wt%. The maximum yield of C4 olefins was obtained at 350° C and 2wt% Co loading.

Different ethanol concentration per minute: under the condition of 200mg 1wt%Co/ Sio2-200mg HAP, the data of ethanol concentration 1.68mL /min and ethanol concentration 0.9mL /min were analyzed. According to Figure 4, it can be seen that different ethanol concentration per minute has little effect on C4 olefin yield.

4. Evaluation of Model

4.1 Advantages

All the models in this paper are established based on the analysis and classification of a large amount of data in the attachment. The data graph and line graph can be used for more intuitive and clear observation. And find the law between data, make the model concise and reliable and more close to the reality.

4.2 Disadvantages

Due to the limited data used in this study, it is impossible to further evaluate the accuracy of the model, which has certain limitations and errors.

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