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# Research based on the factors affecting the preparation of olefin

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***Abstract:*** *The demand for olefin is increasing in countries. At present, prince's principle is mainly used for catalytic coupling ethanol to prepare olefin. This method is cheaper and greener, but there are many problems in the process of preparing olefin. The influence of temperature on ethanol conversion and C4 olefins selectivity was studied by nonlinear regression simulation [1]. Then, the grey correlation degree analysis was used to establish the grey prediction model, and the ranking of the influence of each factor on ethanol conversion was temperature, ethanol concentration, etc., and the ranking of the influence of each factor on C4 olefins selectivity was mass[2], HAP total mass, ethanol flow rate, etc. Finally, the optimum temperature and catalyst combination of olefin preparation were analyzed.*

***Keywords:*** *regression simulation, grey correlation, olefin preparation*

## 1. Background

With the continuous development of economy, the national demand for olefin is increasing day by day. The traditional way to produce olefin is mainly through petroleum catalytic cracking, steam cracking process and methanol/dimethyl ether dehydration condensation. Ethanol, as a very important renewable resource being studied, can get our C4 olefin through catalytic coupling. This reaction is of great significance for industrial production. It not only solves the problem of unbalanced supply and demand of petroleum, but also protects the environment, as ethanol has a lower cost compared with petroleum.

## 2. Modeling and solving of problem 1

### *2.1 Model preparation*

Ethanol conversion and C4 olefin selectivity at different temperatures of each catalyst combination were substituted into the algorithm, with temperature as the horizontal coordinate and ethanol conversion and C4 olefin selectivity as the vertical coordinate. From the images shown by the algorithm, by observing the data inserted in each group, we found that they were all roughly distributed near a straight line. It should be a linear regression problem to guess the relationship between ethanol conversion and C4 olefins selectivity and temperature [3].

### *2.2 Model Establishment*

The unitary nonlinear curve of ethanol conversion rate of each group was obtained through algorithm fitting, as shown in the figure 1.

First combining the given data, we can obtain $\bar{x}$ and $\bar{y}$ by using the following

Formula:

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} \tag{1}$$

$$\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n} \tag{2}$$

Then we can obtain a, B and unary linear regression expressions respectively by using the previous request.

$$a = \bar{y} - b\bar{x} \tag{3}$$

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$$b = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2} \tag{4}$$

$$\hat{Y} = a + bX \tag{5}$$

***2.3 Model Solution***

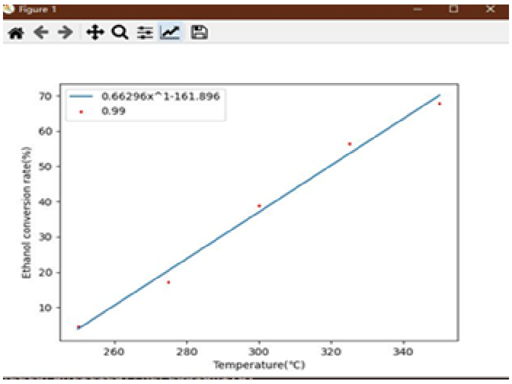
(1) Obtain by using formulas (1) and (2): $\bar{x} = 300, \bar{y} = 37$

Then we get a, b and the expression as follows:

$$a = 0.66296, b = -161.896$$

$$\hat{Y} = 0.66296X - 161.896 \tag{6}$$

(2) Model testing: Through the data of multiple catalyst groups, it is concluded that most of the data have nonlinear regression model, so it is necessary to use nonlinear regression model to solve:



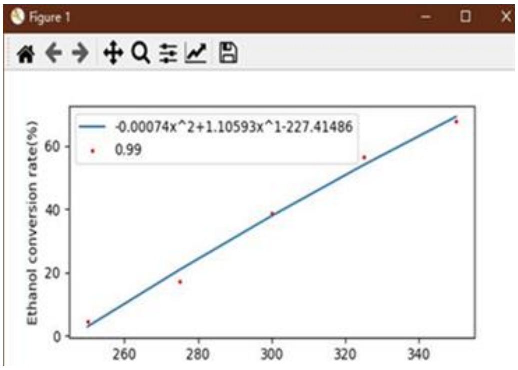




*Figure 1: Ethanol conversion curve with tep*  *Figure 2: Ethanol conversion curve with tep*

1) Two-dimensional scatter point for arbitrary function least square fitting:

$$\rho(y, \hat{y}) = \sqrt{R^2} \tag{7}$$

2) Relation between correlation coefficient and R^2 in least squares:

$$\begin{aligned}
\rho(y_i, \hat{y}_i) &= \frac{\operatorname{cov}(y_i, \hat{y}_i)}{\sqrt{\operatorname{var}(y_i)\operatorname{var}(\hat{y}_i)}} \\
&= \frac{\sum_{i=1}^{n}(y_i - \bar{y})(\hat{y}_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2 \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}} \\
&= \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i + \hat{y}_i - \bar{y})(\hat{y}_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2 \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}} \\
&= \frac{\sum_{i=1}^{n}(y_i - \bar{y}_i)(\hat{y}_i - \bar{y}) + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2 \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}} \\
&= \frac{0 + \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2 \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}} \\
&= \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}} \\
&= \sqrt{\frac{SSR}{SST}} \\
&= \sqrt{R^2}
\end{aligned} \tag{8}$$

Through the above analysis, the nonlinear regression fitting of the above data is obtained as shown in the figure 2.

The fitting equation is obtained:

$$y = -0.00074x^2 + 1..10593x - 227.41486 \tag{9}$$
$$R^2 = 0.991102$$

## 3. Modeling and solving of problem 2

### *3.1 Model preparation*

Because there are so many factors between the two systems, it is necessary to analyze which of the various subfactors influencing the problem are primary and secondary. The grey prediction model is established by using the method of grey correlation degree analysis, and the correlation degree of each sub-factor to the studied index is analyzed and compared according to the dynamic change process of the influence of factors between systems on the problem[4].

### *3.2 Model Establishment*

Grey prediction model is to analyze the correlation degree between the factors of the system, process the data and establish a differential equation model, and then get the influence correlation coefficient, and finally predict the development trend.

(1) Define reference sequence and comparison sequence

Reference sequence and comparison sequence are data sequences that reflect the characteristics of problem behavior and the factors affecting problem behavior respectively.

(2) Dimensionless data processing

The following formula is adopted for dimensionless processing of each sequence:

$$x = (x(1), x(2), \dots, x(n)) \tag{10}$$

$$y = (1, \frac{x(2)}{x(1)}, \dots, \frac{x(n)}{x(1)}) \tag{11}$$

(3) Find the grey correlation coefficient

$$\xi_{0i} = \frac{\Delta(min) + \rho\Delta(max)}{\Delta_{0i}(k) + \rho\Delta(max)} \tag{12}$$

(4) Solving the correlation degree

The correlation degree $r_i$ is calculated by the following formula:

$$r_i = \frac{1}{N}\sum_{k=1}^{N} \xi_i(k) \tag{13}$$

(5) Sorting correlation degree

The degree of correlation can be analyzed and described by sorting the correlation degree in order to compare the influence of different catalyst combinations and temperatures on ethanol conversion and C4 olefins selectivity.

### *3.3 Model Solution*

The correlation degree R of each sub-factor and parent factor was obtained through grey correlation correlation analysis, and the results are shown in the figure below:

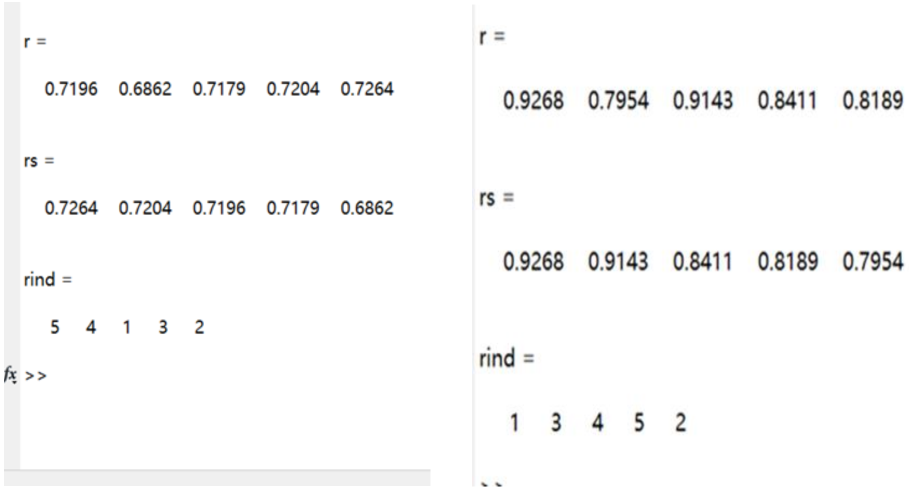



*Figure 3: Correlation of ethanol conversion and selectivity with catalyst factors and temperature*

## 4. Modeling and solving of problem 3

### *4.1 Selection of temperature*

In all the combinations, temperature and C4 selectively satisfy the open-down quadratic function there are three combinations A1,A3 and A13. Their equations obtained by regression analysis and the temperatures at which maximum C4 selectivity was achieved were:

$$\text{A1:}\ -0.00211x^2 + 1.42225x - 190.78343 \quad X_{max} \tag{14}$$

$$\text{A3:}\ -0.00095x^2 + 0.92442x - 171.07588 \quad X_{max} \tag{15}$$

$$\text{A13:}\ -0.00028x^2 - 0.34245x - 64.33291 \quad X_{max} \tag{16}$$

Let X0 be the temperature at which the C4 selectivity of all three equations is the highest relative to each other, then only the maximum positive root of the equation with the three equations standing together is required. set$A = A1(X') + A2(X') + A3(X')$

$$A = -0.00334X'^2 + 2.68912X' + 426.19222 \tag{17}$$

The optimum temperature can be obtained from the properties of the quadratic function: $X_0 = 402.5$

And the same goes for the optimum temperature for ethanol: $X_1 = 1059.2$

Since $X_1$ is much larger than $X_0$, and the correlation between temperature and ethanol obtained through the second question is obviously smaller than that between temperature and C4 selectivity, $X_1$ is omitted.

In conclusion, under the same experimental conditions, 402.5 degrees Celsius was selected as the temperature for the highest C4 olefin yield.

### *4.2 Selection of catalyst combination*

The correlation of various catalyst factors on ethanol conversion and C4 selectivity was obtained by grey correlation analysis. The results show that the selective correlation between THE total mass of $Co/SiO_2$ and C4 is highest $r_0 = 9.268$, followed by the selective correlation between the total mass of HAP and C4 $r_1 = 9.143$.The correlation between the mass ratio of $Co/SiO_2$ and HAP is$r_2 = 0.8401$, so the mass ratio of $Co/SiO_2$ and HAP is not considered as a factor in the selection of catalyst.

In the analysis of the combined correlation degree between ethanol conversion and catalyst, the correlation degree between temperature and ethanol conversion is $r_3 = 0.7264$, and the correlation degree between ethanol flow rate and ethanol conversion is $r_4 = 0.7204$. Therefore, the quality of $Co/SiO_2$ and HAP are mainly considered in the selection of catalyst combination.

Since the mass of $Co/SiO_2$ and HAP are positively correlated with the selectivity of C4 and the conversion of ethanol respectively, the mass of $Co/SiO_2$ and HAP in the catalyst combination should

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be increased as much as possible under experimental conditions.

### *4.3 Temperature below 350 degrees, catalyst combination with temperature selection*

The optimal temperature is 402.5 degrees Celsius, so temperatures below 350 degrees Celsius should be raised as high as conditions permit. As for the selection of catalysts, the correlation between temperature and catalyst is not high, on the basis of the second point, the selection of catalysts can be the same.

## 5. Evaluation of Model

### *5.1 Advantages*

(1) The nonlinear regression model is simple and common, which can calculate the degree of fit and correlation, and also measure the relationship between different variables.

(2) The grey prediction model does not need a large number of samples, the calculation workload is small, and the accuracy of the grey prediction model is high

### *5.2 Disadvantages*

(1) The regression model algorithm is relatively low-level, and the regression equation hypothesis is relatively strict.

(2) The shortcoming of grey prediction model is that the accuracy is not very high.

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