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Research based on the optimal strategy model for the preparation of C4 olefin by ethanol coupling

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Abstract: In this paper, according to different conditions, establish the corresponding model to fit the data, analyze the data results to find the relationship between independent variables and dependent variables, and study the relationship between substances in the chemical reaction[1]. First of all, the linear correlation between data is not high through Pearson coefficient calculation, and the use of linear calculation has a large error, so it is not reference. Then a nonlinear regression model was established, and the relationship between ethanol conversion, C4 olefins selectivity and temperature was obtained by using exponential function fitting data. Finally, according to TOPSIS method, the similarity with the ideal scheme is used as the basis to obtain the optimal solution and the worst solution.

1. Background

C4 olefin is an important chemical raw material,which can be converted into ethanol through chemical reaction under given conditions such as catalyst combination and temperature.Current to ethanol conversion generated C4 hydrocarbon research mainly related conditions in the lab,can reveal the ethanol conversion to a certain extent to generate needed for C4 olefin catalysts,temperature conditions,such as the rule,but difficult to lack of the corresponding mechanism model, the need for laboratory under the condition of limited response analysis,study the mathematical model of the conversion of ethanol generates C4 olefin .Thus it can better guide industrial practice.

2. Modeling and solving of problem 1

2.1 Model Establishment

In order to simplify the problem, Pearson coefficients of ethanol conversion and temperature, C4 olefins selectivity and temperature were obtained, showing positive correlation. Population mean, covariance and Population Pearson coefficient are:

$$E(X)=\frac{\sum_{i=1}^{n} X_i}{n}, E(Y)=\frac{\sum_{i=1}^{n} Y_i}{n} \tag{1}$$

$$\mathrm{Cov}(X,Y)=\frac{\sum_{i=1}^{n}(X_i-E(X))(Y_i-E(Y))}{n} \tag{2}$$

$$\rho_{XY}=\frac{\mathrm{Cov}(X,Y)}{\sigma_X\sigma_Y}=\frac{\sum_{i=1}^{n}\frac{(X_i-E(X))(Y_i-E(Y))}{\sigma_X\sigma_Y}}{n} \tag{3}$$

Pearson's correlation coefficient measures the linear correlation. For the correlation coefficient r between x and y: x and y are positively correlated, 0<r<1; x and y are negatively correlated, -1<r<0.

2.2 Model solving

The Pearson coefficient was used to fit the function with the same feature to find the relationship. Meanwhile, SSE, MSE, RMSE and R-Square indexes were calculated to judge the degree of data fitting.

(1) SSE: This statistical parameter calculates the sum of squares of errors at corresponding points of fitted data and original data:

$$SSE=\sum_{i=1}^{n} w_i(y_i-\widehat{y_i})^2 \tag{4}$$

(2) MSE: This statistical parameter is the mean of the sum of squares of the errors of the corresponding points between the predicted data and the original data:

$$MSE=SSE/n=\frac{1}{n}\sum_{i=1}^{n} w_i(y_i-\hat{y}_i)^2 \tag{5}$$

(3) RMSE: This statistical parameter is the square root of MSE:

$$RMSE=\sqrt{MSE}=\sqrt{SSE/n}=\sqrt{\frac{1}{n}\sum_{i=1}^{n} w_i(y_i-\hat{y}_i)^2} \tag{6}$$

(4) R-Square: Before determining the coefficient, we need to introduce the other two parameters SSR and SST.

a) SSR: the sum of squares of the difference between the predicted data and the mean value of the original data, and the formula is as follows:

$$SSR=\sum_{i=1}^{n} w_i(\hat{y}_i-\bar{y}_i)^2 \tag{7}$$

b) SST: the sum of squares of the difference between the original data and the mean value, and the formula is as follows:

$$SST=\sum_{i=1}^{n} w_i(y_i-\bar{y}_i)^2 \tag{8}$$

$$R-\text{ square }=\frac{SSR}{SST}=\frac{SST-SSE}{SST}=1-\frac{SSE}{SST} \tag{9}$$

The "deterministic coefficient" represents the quality of a fit through changes in data. Its normal value range is [0 1], and the closer it is to 1, the stronger the variable of the equation is in explaining y, and the better the model fits the data.

3. Modeling and solving of problem 2

3.1 Model based on TOPSIS

TOPSIS method is used to study the sequential optimization technology of similarity with the ideal scheme.Through TOPSIS, it can calculate the size of the data, analyze the advantages and disadvantages of the data, and find out the positive and negative ideal solutions and the distance between the positive and negative ideal solutions combined with the size of the data, so as to screen out the best scheme[2].

(1) Data normalization: Several major variables affecting C4 olefin yield were identified:

temperature, Hap, ethanol concentration, and Co load. Because of Hap, the temperature is a positive impact on C4 olefin selectivity, Co load will produce negative influence, so will take reciprocal Co load data[3], then the above five variables to normalization of sum of squares (SSN) processing,its purpose is to put all the data values in the size of the unity,making the analysis process will not appear larger error, processing formula is:

$$x_i' = \sqrt{\sum_1^n x_i^2} \tag{10}$$

(2) Build the raw data matrix:Among them,n is 114 plans,namely,114 data given in the question.Temperature,Hap,ethanol concentration and Co load are selected as evaluation indexes to establish a matrix for 114 data.

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1\rho} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \cdots & \cdots & \cdots & \cdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}_{n\times p} \quad Z = \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1p} \\ z_{21} & z_{22} & \cdots & z_{2p} \\ \cdots & \cdots & \cdots & \cdots \\ z_{n1} & z_{n2} & \cdots & z_{np} \end{bmatrix}_{n\times p} \tag{11}$$

(3) The optimal value vector and the worst value vector are constituted by the inferior values of different catalyst combinations and temperatures respectively.

$$\begin{cases} Z^+ = \left(z_1^+, z_2^+, \cdots, z_p^+\right); Z^- = \left(z_1^-, z_2^-, \cdots, z_p^-\right) \\ z_j^+ = max\left\{z_{1j}, z_{2j}, \cdots, z_{nj}\right\}, j = 1,2, \cdots, p \\ z_j^- = min\left\{z_{1j}, z_{2j}, \cdots, z_{nj}\right\}, j = 1,2, \cdots, p \end{cases} \tag{12}$$

(4) Calculate the vertical shortest distance between the optimal and the worst values of different catalyst combinations and temperatures.

$$\begin{cases} D_i^+ = \sqrt{\sum_{j=1}^{\rho} \left(z_{ij} - z_j^+\right)^2}, \\ D_i^- = \sqrt{\sum_{j=1}^{\rho} \left(z_{ij} - z_j^-\right)^2} \end{cases} \tag{13}$$

(5) Evaluate the relative proximity of different catalyst combinations and temperatures to the optimal scheme.

$$C_i = \frac{D_i^-}{D_i^+ + D_i^-}, i = 1,2, \cdots, n \tag{14}$$

(6) Sort according to proximity.The greater the value of C, the better the scheme.

3.2 Evaluation calculation based on TOPSIS

TOPSIS method firstly finds the positive and negative ideal solutions of the evaluation index, then calculates the distance values D+ and D- between each evaluation object and the positive and negative ideal solutions, and finally calculates the proximity of each evaluation object to the optimal scheme.

Table 1: TOPSIS evaluates the calculation results

Item	D+	D-	C	Sorting result
Object 10	0.221	0.299	0.574	5
Object 16	0.217	0.417	0.657	2
Object 17	0.217	0.406	0.652	3
Object 23	0.243	0.359	0.596	4
Object 34	0.120	0.396	0.768	1

The results showed that under all the conditions of temperature, the evaluation object 34 was the best scheme, that is, the temperature was 400 degrees, the concentration of 200mg 5wt%Co/ Sio2-200mg HAP-ethanol was 1.68 mL /min.

Table 2: TOPSIS evaluates the calculation results (Below 350 degrees Celsius)

Item	D+	D-	C	Sorting result
Object 8	0.178	0.646	0.784	1
Object 12	0.271	0.438	0.618	2
Object 4	0.289	0.418	0.591	3
Object 16	0.32	0.419	0.566	4
Object 7	0.383	0.348	0.476	5

The results show that when the temperature is below 350 degrees Celsius, the evaluation object 8 is the best scheme, namely, the temperature is 300 degrees, 200mg 2wt%Co/ Sio2-200mg HAP-ethanol concentration is 1.68mL /min.

4. Evaluation of Model

4.1 Advantages

(1) The model fully considers the random correlation of data and calculates Pearson's coefficient. More accurate prediction model, and on this basis, testing a variety of functional models, r-value fitting degree 0.9997.

(2) According to TOPSIS method, the similarity with the ideal scheme is used as the basis to obtain the optimal solution and the worst solution, which makes the model more integrated and clearer.

4.2 Disadvantages

(1) The operation scale of the model is large and time-consuming.

(2)The model has not carried out in-depth research on the intelligent optimization algorithm.

References

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