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Study on Preparation of Olefins by Ethanol Coupling based on Grey Relational Analysis

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Abstract: As an important chemical raw material, C4 olefin is widely used in daily life. In this paper, the correlation between physicochemical factors and temperature and the conversion rate of ethanol and the selectivity of 6 C4 olefins in 21 kinds of catalyst combinations were investigated and the correlation between them was analyzed. Then based on the size of the grey correlation value to measure the influence between factors and get the order of influencing factors.

1. Introduction

With the rapid development of economy, people have more and more demand for crude oil products, and their awareness of environmental protection has gradually improved. In daily life, C4 olefins are widely used in the production of chemical products and medicine. Under the premise of less or zero pollution, the efficient preparation of C4 olefins is of great significance and value. Ethanol is used as the raw material of C4 olefins. In the preparation process, the combination of catalysts and temperature will affect the selectivity and yield of C4 olefins, which seriously affects the preparation of C4 olefins. Through a series of experiments on different catalyst combinations at different temperatures, and then according to the experimental results, the conditions for the highest C4 olefin yield were found.

2. Pearson correlation coefficient model

Correlation coefficient: a general term for a class of indicators that measure the correlation between variables. In terms of parameter statistics, Pearson product moment correlation coefficient [2] (Pearson): that is, the ratio between covariance and two variable standard deviation is dimensionless and standardized covariance. Covariance: the average of the product of two variables and their mean deviation. It is a measure of their relationship.

Overall covariance:

$$\sigma_{xy} = \frac{\sum(x_i-\mu_x)(y_i-\mu_y)}{N} \tag{1}$$

Sample covariance:

$$S_{xy} = \frac{\sum(x_i-\overline{x})(y_i-\overline{y})}{n-1} \tag{2}$$

According to the calculation formula of sample correlation coefficient:

$$r = \frac{n\sum xy - \sum x \sum y}{\sqrt{n\sum x\text{^}2 - (\sum x)\text{^}2} \cdot \sqrt{n\sum y\text{^}2 - (\sum y)\text{^}2}} \quad (3)$$

The value range of correlation coefficient is: -1≤R≤1. Positive indicates positive correlation and negative indicates negative correlation. Use the correlation coefficient to judge the closeness of the correlation [3]

Table 1: Correlation coefficient and the closeness of correlation

The value of correlation coefficient	Linear correlation degree
|r|=0	Totally irrelevant
0<|r|≤0.3	Weak correlation
0.3<|r|≤0.5	Low correlation
0.5<|r|≤0.8	Significant correlation
0.8<|r|≤1	Highly correlated
|r|=1	Complete correlation

3. Relationship between 7 indexes and temperature

In this paper, the correlation between the conversion rate of ethanol, the selectivity of six C4 olefins and temperature was studied. Without considering the selection of catalyst combination, it can be found that some of the variable indexes are not linear. Therefore, we calculate the Pearson correlation coefficient corresponding to each variable index, and compare the value of the Pearson correlation coefficient with the matrix scatter diagram as the basis for explaining the correlation between the two variable indexes.

Table 2: Pearson correlation coefficient between ethanol conversion and selectivity of six C4 olefins and temperature

	Temperature	Ethylene selectivity (%)	Selectivity of C4 olefins (%)	Selectivity of acetaldehyde (%)	Carbon number 4-12 fatty alcohol selectivity (%)	Selectivity of methyl benzaldehyde and methyl benzyl alcohol (%)	Selectivity of other products (%)	Ethanol conversion (%)
Temperature	1	.664**	.700**	0.101	-.703**	.269**	.708**	.771**
Ethylene selectivity (%)	.664**	1	.579**	.361**	-.771**	-0.004	.414**	.607**
Selectivity of C4 olefins (%)	.700**	.579**	1	-0.168	-.663**	0.147	.770**	.735**
Selectivity of acetaldehyde (%)	0.101	.361**	-0.168	1	-.603**	-.184*	-.189*	-0.065
Carbon number 4-12 fatty alcohol selectivity (%)	-.703**	-.771**	-.663**	-.603**	1	-0.076	-.556**	-.594**
Selectivity of methyl benzaldehyde and methyl benzyl alcohol (%)	.269**	-0.004	0.147	-.184*	-0.076	1	0.133	.286**
Selectivity of other products (%)	.708**	.414**	.770**	-.189*	-.556**	0.133	1	.682**
Ethanol conversion (%)	.771**	.607**	.735**	-0.065	-.594**	.286**	.682**	1

Similarly, the Pearson correlation coefficient between the conversion rate of ethanol and the selectivity of six C4 olefins and temperature can also be calculated by using the above method.

Table 3: Correlation coefficients between ethanol conversion, selectivity of six C4 olefins and temperature under different catalysts

	Ethanol conversion (%)	Ethylene selectivity (%)	Selectivity of C4 olefins (%)	Selectivity of acetaldehyde (%)	Carbon number 4-12 fatty alcohol selectivity (%)	Selectivity of methyl benzaldehyde and methyl benzyl alcohol (%)	Selectivity of other products (%)
A1	0.965**	0.943*	0.887*	0.928*	-0.963**	0.900*	0.538
A2	0.995**	0.892*	0.914*	0.980**	-0.938*	0.707	0.979**
A3	0.982**	0.929**	0.955**	0.933**	-0.973**	-0.634	0.896**
A4	0.998**	0.953**	0.958**	0.970**	-0.962**	0.903*	0.970**
Average	0.948	0.893	0.953	0.481	-0.904	0.37	0.927

Among the physical and chemical factors of 21 catalyst combinations, the correlation coefficient values of ethanol conversion, C4 olefin selectivity and selectivity of other products are between [0.8,1] (except that A1 combination in the selectivity of other products is 0.538). Therefore, it can explain the ethanol conversion, C4 olefin selectivity and selectivity of 20 catalyst combinations of A2 ~ B7 There is a strong positive correlation between the selectivity of C4 olefins and other products and temperature. In the correlation coefficient of fatty alcohol selectivity with carbon number of 4-12, the correlation coefficient value of a11 combination is 0. Therefore, it can be considered that the carbon number of a11 combination is 4-12, and there is no correlation between fatty alcohol selectivity and temperature. In the correlation coefficient of fatty alcohol selectivity with carbon number of 4-12, the correlation coefficient value of a11 combination is 0. Therefore, it can be considered that the carbon number of a11 combination is 4-12, and there is no correlation between fatty alcohol selectivity and temperature. The absolute values of A5, A9, B6 and B7 are all between [0,0.3], which can be considered to have a weak correlation with temperature; The absolute values of A8 and A10 are between [0.3, 0.5], which can be considered to have low correlation with temperature

4. Grey correlation analysis

The four components and temperature of the catalyst have different effects on ethanol conversion and C4 olefin selectivity. We conduct grey correlation analysis on the two variables of each catalyst component and temperature, and extract the grey correlation coefficient of each component under different content / concentration and temperature.

4.1 Data standardization processing

Firstly, the mean value of the data is calculated, that is, the average value of each group of data at each distribution point is obtained. Then the data are dimensionless processed by the extreme value method, that is, divide each group of data by the maximum value of the corresponding group, and finally get the new data group as the standardized sequence, as shown in the table below:

Table 4: CO load and standardized conversion of physical and chemical factors

Co load	Ethanol conversion (%)	Selectivity of C4 olefins (%)
0.1	1	0.876691644
0.2	0.554752626	0.74520856
0.4	0.974242987	1
1	0.640520943	0.648214265

4.2 Calculate absolute value difference

The absolute difference is calculated according to the original research data, that is, the absolute difference table is as follows:

Table 5: Absolute difference between Co load and physicochemical factors

CO load	
Ethanol conversion (%)	Selectivity of C4 olefins (%)
0.9	0.776691644
0.354752626	0.54520856
0.574242987	0.6
0.359479057	0.351785735

4.3 Solution of model

The sequence and correlation coefficient are calculated by the following formula:

$$\zeta_i(k) = \frac{\min_i \min_k |x_0(k) - x_i(k)| + \rho \cdot \max_i \max_k |x_0(k) - x_i(k)|}{|x_0(k) - x_i(k)| + \rho \cdot \max_i \max_k |x_0(k) - x_i(k)|} \tag{4}$$

The average value of the correlation coefficient of each period of the comparison series and the reference series is used to quantitatively reflect the correlation degree of the two series, and the calculation formula is:

$$\gamma_{0i} = \frac{1}{n^n} \sum_{k=1}^{n} \gamma_{0i}, i = 1,2, \dots, m \tag{5}$$

According to the correlation order of its numerical value, the close relationship between the composition of different catalysts and the conversion of ethanol and the selectivity of C4 olefins was judged, and the main factors affecting the quantitative change were screened out.

Table 6: Correlation degree of five variables on ethanol conversion and C4 olefin selectivity

	Evaluation item	Correlation degree
Co/SiO2 content.	Ethanol conversion (%)	0.675
	Selectivity of C4 olefins (%)	0.79
Co load	Selectivity of C4 olefins (%)	0.786
	Ethanol conversion (%)	0.75
Ethanol concentration	Ethanol conversion (%)	0.614
	Selectivity of C4 olefins (%)	0.614
HAP content	Ethanol conversion (%)	0.658
	Selectivity of C4 olefins (%)	0.794
Temperature	Ethanol conversion (%)	0.618
	Selectivity of C4 olefins (%)	0.575

5. Conclusion

In this paper, the Pearson correlation coefficients of 21 kinds of catalysts at each temperature are calculated by using mathematical statistical method, person correlation coefficient and grey correlation analysis. It is concluded that there is a high negative correlation between time and ethanol conversion and carbon number of 4-12 fatty alcohols, and a high positive correlation between time

and ethylene selectivity and acetaldehyde selectivity. Then, according to the different combinations of catalysts and temperature, the grey correlation value is used to measure the influence of factors. The effect on ethanol conversion can be obtained by numerical order: Co loading > Co/SiO2 content > HAP content > temperature > ethanol concentration, and for C4 olefin selectivity: temperature > ethanol concentration > Co loading > Co/SiO2 content > HAP content.

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