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Study on Influencing Factors of Ethanol Catalytic Coupling Process Based on Multivariable Regression

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Abstract: *C4 olefins are widely used in the production of chemical products and medicine. Ethanol is the raw material for the production of C4 olefins. Traditional production methods use fossil energy as raw materials. The purpose of this paper is to explore the selection of catalyst combination and temperature for the preparation of C4 olefins by ethanol catalytic coupling. Firstly, correspondence analysis model was used to explore the relationship between ethanol conversion, C4 olefin selectivity and temperature. It is concluded that the ethanol conversion and C4 olefin selectivity increase with the increase of temperature. Then, the multivariable regression method is used to solve the relationship between multiple independent variables and multiple dependent variables through the partial least square method. Different catalyst combinations and temperatures are analyzed to obtain the regression equation of ethanol conversion and C4 olefin selectivity. The effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity are intuitively observed. Temperature, solution quality and HAP are positively correlated,* Co/SiO_2 *and ethanol concentrations were negatively correlated with them.*

Keywords: *C4 olefin selectivity; Ethanol conversion; Partial least square method*

1. Introduction

C4 olefins are widely used in the production of chemical products and medicine. Ethanol is the raw material for the production of C4 olefins. Traditional production methods use fossil energy as raw materials. However, with the shortage of fossil energy output and the aggravation of environmental impact, the energy supply gradually tends to be diversified, and the development of new clean energy is more and more urgent. Through the structural design and preparation of catalysts, to explore the process conditions for the preparation of C4 olefins by ethanol catalytic coupling [1].

2. Construction of temperature effect model

This paper collects the results of various catalyst combinations, and studies the relationship between ethanol conversion, C4 olefin selectivity and temperature for each catalyst combination. If there are n samples and P different indexes are observed for each sample, the original data is:

$$\boldsymbol{A}=\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{np} \end{bmatrix} \tag{1}$$

Starting from the original data matrix A, calculate the corresponding matrix P and the corresponding transformed new data matrix B, and calculate the row contour distribution [2], which is recorded as:

$$R=\left(\frac{a_{ij}}{a_{i\bullet}}\right)_{n\times p}=\left(\frac{p_{ij}}{p_{i\bullet}}\right)_{n\times p}=D_r^{-1}P=\begin{bmatrix} def \\ R_1^T \\ \vdots \\ R_n^T \end{bmatrix} \tag{2}$$

Probability matrix *P*: $P=\frac{1}{T}A=\left(p_{ij}\right)_{n\times p}$

R matrix is obtained by dividing each row of a matrix (or corresponding matrix P) by row sum, which is to eliminate the different influence of "probability" of row points (i.e. sample points). $N(R)=\{R_i, i=1,2,\cdots,n\}$ represents the p-dimensional space point set composed of row images, then the center of gravity C of the point set can be obtained. The different effects of "probability" are obtained by calculating the C matrix (i.e. each column of the a matrix is divided by the column sum), and then the total inertia and χ^2 statistics are calculated. The weighted square distance (or χ^2 distance) between the K and l samples is:

$$D^2(k,l)=\sum_{j=1}^{p}\left(\frac{p_{lj}}{p_{k\bullet}}-\frac{p_{lj}}{p_{l\bullet}}\right)^2 / p_{\bullet j}=\left(R_k-R_l\right)^T D_c^{-1}\left(R_k-R_l\right) \tag{3}$$

In this paper, the sum of the weighted square distances from n sample points (i.e. line points) to the center of gravity C is defined as the total inertia of the line image point set (NR).

$$\begin{aligned} Q&=\sum_{i=1}^{n}p_i D^2(i,c)=\sum_{i=1}^{n}p_{i\bullet}\sum_{j=1}^{p}\frac{1}{p_{-j}}\left(\frac{p_{ij}}{p_{i\bullet}}-p_{\bullet j}\right)^2 \\ &=\sum_{i=1}^{n}\sum_{j=1}^{p}\frac{p_i}{p_{\bullet j}}\frac{\left(p_{ij}-p_{i\bullet}p_{\circ j}\right)^2}{p_{i\bullet}^2}=\sum_{i=1}^{n}\sum_{j=1}^{p}\frac{\left(p_{ij}-p_{i=}p_{\cdot j}\right)^2}{p_i p_{\bullet j}}=\sum_{i=1}^{n}\sum_{j=1}^{p}b_{ij}^2=\frac{\chi^2}{T} \end{aligned} \tag{4}$$

Set the eigenvalue as $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_m\geq 0$, and the corresponding standardized eigenvector is $\eta_1,\eta_2,\cdots,\eta_m$. In practical application, the cumulative contribution rate is often used:

$$\frac{\lambda_1+\lambda_2+\cdots+\lambda_l}{\lambda_1+\cdots+\lambda_l+\cdots+\lambda_m}\geq 0.80(\&0.70,0.85) \tag{5}$$

Then calculate the row contour coordinate *G* and column contour coordinate *F*, and then analyze and calculate the "factor load matrix" of *R*-type and *Q*-type factor analysis. Draw the point plan on the same two-dimensional plane with row contour coordinate G and column contour coordinate F (take m=2), and obtain the total inertia Q and χ^2 statistics.

3. Model solution of the effect of temperature on ethanol conversion and C4 olefin selectivity

Table 1: A1 group inertia and χ^2 decomposition

Singular value	Principal inertia	χ^2	Contribution rate	Contribution rate
0.257796005	0.06645878	138.1924041	0.945950856	0.945950856
0.046024314	0.002118237	4.404599741	0.030150245	0.976101101
0.036113691	0.001304199	2.711911864	0.018563505	0.994664606
0.019360883	0.000374844	0.779438989	0.005335394	1
3.21E-17	1.03E-33	2.14E-30	1.46E-32	1

According to Table 1, the total χ^2 statistic is 97 60% can be explained by the first two dimensions. It indicates that the relationship between row points and column points can be expressed in two dimensions.

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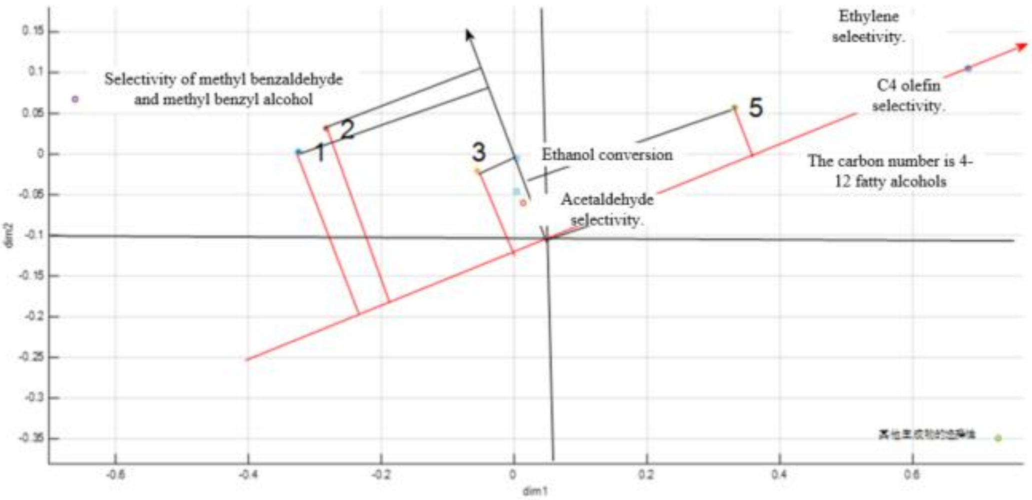

Figure 1: Scatter diagram of group A1 row points and column points

It can be concluded from Figure 2 and table 1 that in the A1 catalyst combination, the ethanol conversion and C4 olefin selectivity increase with the increase of temperature, and begin to decrease until the temperature reaches 325℃. However, the ethanol conversion is lower than other catalyst combinations, and the C4 olefin selectivity is higher than other catalyst combinations. Similarly, we can get the scatter diagram and card room solution table of other groups, which shows that the ethanol conversion and C4 olefin selectivity increase with the increase of temperature.

4. Construction of multivariate model based on partial least squares regression

Considering the different combinations of catalysts, the different combinations of catalysts are subdivided into solution weight, Co / SiO2, HAP and ethanol concentration [4]. These four variables and temperature involve a total of five independent variables. The effects on ethanol conversion and C4 olefin selectivity should be discussed. Ethanol conversion and C4 olefin selectivity are two dependent variable factors. X1, X2, X3, X4 and X5 respectively represent the independent variable index temperature, solution weight, Co / sio2hap and ethanol concentration, Y1 and Y2 respectively represent the independent variable index ethanol conversion and C4 olefin selectivity.

Record the independent variable observation data matrix as $A=\left(a_{ij}\right)_{109\times5}$ and the observed data and the dependent variable are recorded as $B=\left(b_{ij}\right)_{109\times5}$.

4.1. Data processing

Convert each index value a_{ij} into a standardized index value a_{ij}.

$$\tilde{\alpha}_{ij}=\frac{\alpha_{ij}-\mu_j^{(1)}}{s_j^{(1)}}, i=1,2,\ldots,109,\ j=1,2,3,4,5 \tag{6}$$

$\mu_j^{(1)}=\frac{1}{109}\sum_{i=1}^{109}a_{ij};s_j^{(1)}=\sqrt{\frac{1}{109-1}\sum_{i=1}^{109}\left(a_{ij}-\mu_j^{(1)}\right)^2}$, $j=1,2,3,4,5$, $\mu_j^{(1)}$ is the sample mean, $s_j^{(1)}$ is the standard deviation of the sample. Treat $\tilde{b}_{ij}$ in the same way, the correlation coefficient matrix is established.

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Table 2: Correlation matrix

	Temperature (x_1)	Solution weight (x_2)	Co/SiO2(x_3)	HAP(x_4)	Ethanol concentration (x_5)	Ethanol conversion (y_1)	C4 olefin selectivity (y_2)
Temperature (x_1)	1	-0.00219	-0.01477	-0.00219	-0.03932	0.77753	0.72407
Solution weight (x_2)	-0.00219	1	0.20031	0.98937	-0.29129	0.38592	0.36125
Co/SiO2(x_3)	-0.01477	0.20031	1	0.20031	0.14863	0.0326	-0.18662
HAP(x_4)	-0.00219	0.98937	0.20031	1	-0.29129	0.39233	0.34952
Ethanol concentration (x_5)	-0.03932	-0.29129	0.14863	-0.29129	1	-0.32669	-0.09209
Ethanol conversion (y_1)	0.77753	0.38592	0.0326	0.39232	-0.32669	1	0.73160
C4 olefin selectivity (y_2)	0.72407	0.36125	-0.18662	0.34952	-0.09209	0.7316	1

4.2. Solving correlation coefficient matrix

It can be seen from table 2 that temperature is positively correlated with ethanol conversion and C4 olefin selectivity, solution weight is positively correlated with ethanol conversion and C4 olefin selectivity, Co / SiO2 is positively correlated with ethanol conversion and negatively correlated with C4 olefin selectivity. HAP is positively correlated with ethanol conversion and C4 olefin selectivity. Ethanol concentration was negatively correlated with ethanol conversion and C4 olefin selectivity.

4.3. Solution of regression equation

Firstly, the corresponding pairs of components are obtained by MATLAB [3], and then the regression equation is solved, such as u_1, v_1:

$$\begin{cases} u_1 = -0.0645\tilde{x}_1 - 0.0321\tilde{x}_2 - 0.0061\tilde{x}_3 - 0.03190\tilde{x}_4 + 0.0185\tilde{x}_5 \\ v_1 = -8.7329\tilde{y}_1 - 7.8027\tilde{y}_2 \end{cases} \tag{7}$$

Obtain the regression equation between the time standardized indicators of the four components and the component variables, and obtain the regression equation related to u_1 and u_2.

$$\tilde{x}_1 = -7.0354u_1 - 7.2371u_2 \qquad \tilde{y}_1 = -8.7329u_1 - 2.6619u_2$$

$$\tilde{x}_2 = -7.3068u_1 + 6.7054u_2 \qquad \tilde{y}_2 = -7.8027u_1 - 3.6651u_2$$

$$\tilde{x}_3 = -0.3281u_1 + 3.7686u_2$$

$$\tilde{x}_4 = -7.3066u_1 + 6.7065u_2$$

$$\tilde{x}_5 = 4.33230u_1 - 3.2695u_2$$

$$\tilde{y}_1 = 0.7423\tilde{x}_1 + 0.2144\tilde{x}_2 - 0.1253\tilde{x}_3 + 0.2103\tilde{x}_4 - 0.1022\tilde{x}_5$$

$$\tilde{y}_2 = 0.7499\tilde{x}_1 + 0.1599\tilde{x}_2 - 0.1469\tilde{x}_3 + 0.1549\tilde{x}_4 - 0.0626\tilde{x}_5$$

Then the dependent variable and independent variable are brought into the regression equation to obtain:

$$y_1 = -34.2568 + 0.3270x_1 + 0.0695x_2 - 2.4355x_3 + 0.0682x_4 - 4.4588x_5$$

$$y_2 = -45.3337 + 0.1939x_1 + 0.0304x_2 - 1.6759x_3 + 0.0295x_4 - 1.6035x_5$$

4.4. Model results

It can be concluded that the temperature variable plays a very important role in explaining the two regression equations. However, compared with other factors, the explanatory ability of CO / SiO2 independent variable on ethanol conversion is very low. Solution weight, HAP and ethanol concentration all played a role in the interpretation of the regression equation.

5. Conclusion

In this paper, correspondence analysis and partial least squares were used to study the effects of catalyst combination and temperature on ethanol conversion and C4 olefin selectivity. Firstly, the correspondence analysis model is used to deal with it, and it is concluded that the ethanol conversion and C4 olefin selectivity increase with the increase of temperature. Then the regression equations of ethanol

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conversion and C4 olefin selectivity were obtained based on partial least square method. The effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity were observed intuitively. Temperature, solution quality and HAP were positively correlated, and Co/SiO_2 and ethanol concentration were negatively correlated.

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