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Production of C4 Olefins by Ethanol Coupling based on Linear Regression Equation

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Abstract

As an important chemical raw material, C4 olefins are widely used in the production of chemical products and pharmaceutical intermediates. Ethanol is an important raw material for the preparation of C4 olefins. The experimental results of a given catalyst combination at 350 ℃ for different time were analyzed. The effects of different catalyst combinations on ethanol conversion, C4 olefin selectivity and temperature were investigated. By analyzing and preprocessing the known data, the uniformly divided B-spline curve is generated based on the curve fitting algorithm, and the curve fitting graph and fitting expression are generated. The linear relationship between ethanol conversion, C4 olefin selectivity and temperature was obtained by linear regression equation. Finally, the linear regression equation and fitting diagram are classified and explained.

Keywords

Linear Regression Equation; Ethanol Conversion Ratio; C4 Olefin Yield.

1. Introduction

Currently, C4 olefins are widely used in the production of chemical products and pharmaceuticals. In chemical products, through the use of C4 olefin products, the production capacity and economic benefits of the petrochemical industry can be effectively improved. Therefore, can vigorously develop C4 olefins [1]. As a feedstock for the production of C4 olefins, ethanol is a large chemical product with relatively low price, and can be prepared by microbial fermentation. Consistent with sustainability and regeneration in the concept of sustainable development [2]. Different catalyst combinations and reaction temperatures were designed, and the catalyst combinations and temperatures with better catalytic ethanol conversion ratio performance to C4 olefins were compared for the preparation of C4 olefins from ethanol to prepare C4 olefins with high yields.

Investigate ethanol conversion ratio, C4 olefin selectivity versus temperature for each catalyst combination. Analyze the test results of a given catalyst combination at 350 degrees at different times in one experiment.

2. Problem Analysis

It is a very meaningful problem to study the catalyst combination and temperature for the efficient preparation of C4 olefins from ethanol. It has an important impact on the improvement of the production capacity and efficiency of the petrochemical industry. Due to the uncertainty of catalyst combination and temperature, the laboratory can only draw conclusions by changing catalyst combinations and temperatures and conducting constant tests. Therefore, the main goal of this paper is to fully analyze the existing experimental data and extract useful variables from it .Through these variables, a reasonable and effective catalyst combination and temperature effect evaluation system for the preparation of C4 olefins by ethanol coupling were established. Construction of optimal catalyst combination and temperature influence model based on desired C4 olefin yield, According to the C4 olefin yield corresponding to different catalyst combinations and temperatures, the maximization of the C4 olefin yield is achieved .On the basis of this system, the effects of ineffective catalyst combination and temperature and experimental error were considered.

There are two problems to be solved. On the one hand, the relationship between ethanol conversion ratio, C4 olefin selectivity and temperature was analyzed separately for each catalyst combination. On the other hand, analyze the test results for a given catalyst combination at 350 degrees Celsius over time .Using Matlab, the curve fitting graph and fitting polynomial of ethanol conversion ratio, C4 olefin selectivity and temperature were obtained for each catalyst combination. The linear relationship between ethanol conversion ratio, C4 olefin selectivity and temperature for each catalyst combination was obtained by linear regression equation. After error verification, errors greater than 0.05 need to be optimized. Afterwards, the similar relational expressions and fitting graphs are classified and explained. Finally, plot the fit between selectivity, ethanol conversion ratio, and time for each product.

Model Assumptions:

Ignoring the effects of environmental variables other than catalyst combination and temperature, it is assumed that all experiments given in the appendix were performed under exactly the same ideal environment.

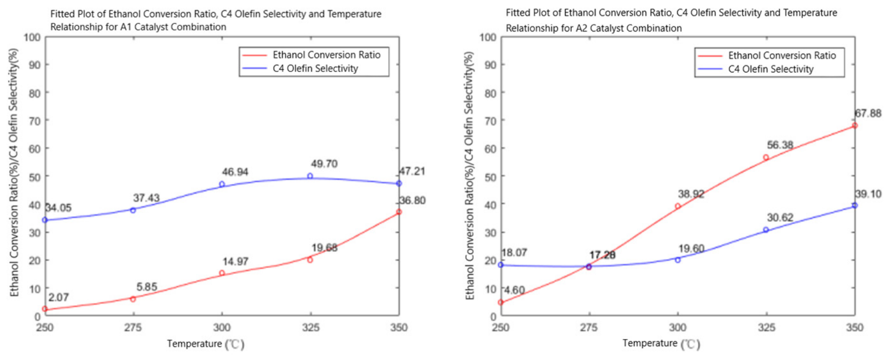
(Note: The following is a description of the symbols)

Table 1. Description of the symbols

Symbol	Meaning
ET	Ethanol Conversion Ratio
T	Temperature
C	C4 Olefin Selectivity
A	Packing Method Ⅰ
B	Packing Method Ⅱ

3. Model Building

3.1. Exploring the Relationship between Ethanol Conversion Ratio, C4 Olefin Selectivity and Temperature



$ET=1.628e{-}05T^3-0.01539T^2+4.99T-538.5$

$C=-3.905e{-}06T^3+0.002325T^2-0.1604T-10.83$

$ET=-8.043e{-}05T^3-0.02916T^2-20.44T+1893$

$C=-3.013e{-}05T^3+0.03023T^2-9.718T+1029$

Figure 1. Fitting Graph and Fitting Polynomial of the Relationship between Ethanol Conversion Ratio, C4 Olefin Selectivity and Temperature in Two Catalyst Combinations

Model:Linear regression,A Curve Fitting Algorithm for Basis Generating Uniformly Partitioned B-Splines.

According to the data given in Annex I, by using Matlab to calculate the relationship between ethanol conversion ratio, C4 olefin selectivity and temperature in each catalyst combination, the fitting graph and fitting relation polynomial are obtained. As it in Figure 1. Polynomials can almost perfectly fit all known data. Therefore, the polynomial in the figure can be regarded as the relational expression of ethanol conversion ratio, C4 olefin selectivity and temperature.

In order to facilitate quantitative analysis, linear regression was used to obtain the relationship between the ethanol conversion ratio, C4 olefin selectivity and temperature of each catalyst combination in Table 2, and it was verified that the errors were all less than 0.05.

Table 2. Relational expressions of ethanol conversion ratio, C4 olefin selectivity and temperature for 21 catalyst combinations

name	Ethanol conversion ratio and temperature	C4 olefin selectivity and temperature
A1	ET=0.3332T-84.074	C=0.1544T-3.242
A2	ET=0.6630T-161.8920	C=0.2216T-41.5460
A3	ET=0.4194T-95.8275	C=0.2612T-59.1949
A4	ET=0.5816T-144.5400	C=0.2266T-52.4106
A5	ET=0.4077T-97.5929	C=0.2297T-57.8127
A6	ET=0.5012T-119.7310	C=0.2027T-50.7483
A7	ET=0.3773T-74.1819	C=0.1869T-44.2622
A8	ET=0.3392T-83.6302	C=0.2423T-57.2566
A9	ET=0.2490T-65.6241	C=0.2538T-59.0950
A10	ET=0.1835T-49.6879	$C=4.752e-06T^3-0.003924T^2+1.073T-95.06$
A11	ET=0.2070T-56.5741	C=0.0519T-13.3074
A12	ET=0.2858T-74.7957	C=0.2049T-47.7272
A13	ET=0.2533T-67.3328	C=0.1628T-35.8893
A14	ET=0.3358T-86.6440	C=0.1381T-35.3522
B1	ET=0.2796T-73.1897	C=0.2397T-56.7277
B2	ET=0.2724T-70.8595	C=0.2441T-61.0731
B3	ET=0.1314T-36.1843	C=0.1202T-28.2944
B4	ET=0.2080T-56.9000	C=0.1023T-22.2081
B5	ET=0.2720T-72.4000	C=0.1462T-34.5994
B6	ET=0.3833T-99.8829	C=0.1903T-45.7573
B7	ET=0.4197T-109.3429	C=0.2337T-56.4513

Let L be the slope of the linear expression for ethanol conversion ratio or C4 olefin selectivity versus temperature. From the value of L, it can be seen that the temperature has an increasing relationship with the ethanol conversion ratio and the C4 alkane selectivity. It can be seen that the higher the temperature, the higher the ethanol conversion ratio and the C4 alkane selectivity. The larger the value of L, the higher the sensitivity of the catalyst combination to temperature.

As it in Table 3. In the catalyst combination named A2, the slope of the linear relationship of ethanol conversion ratio with temperature is 0.6630. It can be seen that under the catalysis of this catalyst combination, the ethanol conversion ratio has the highest sensitivity to temperature. In the catalyst combination named B3, the slope of the linear relationship of ethanol conversion ratio with temperature was 0.1314. It can be seen that under the catalysis of this catalyst combination, the ethanol conversion ratio has the least sensitivity to temperature.

Table 3. Regression expression slope distribution interval relationship between each catalyst combination and ethanol conversion ratio and temperature

Catalyst Combination	Slope Interval
B3	0.1314
A10, A11, B4	[0.1835,0.2080]
A9,A13	[0.2490,0.2533]
A12,B1,B2,B5	[0.2720,0.2858]
A1,A8,A14	[0.3332,0.3392]
A7,B6	[0.3773,0.3833]
A3,A5,B7	[0.4077,0.4197]
A4,A6	[0.5021,0.5816]
A2	0.6630

Table 4. Intervals of Regression Expression Slope Distributions Between Catalyst Combinations and C4 Olefin Selectivity and Temperature

Catalyst Combination	Slope Interval
A11	0.0519
B3,B4	[0.1023,0.1202]
A14,B5	[0.1381,0.1462]
A6,A7,A12,B1	[0.1869,0.2049]
A2,A4,A5	[0.2216,0.2297]
A8,A9,B1, B2, B7	[0.2337,0.2538]
A3	0.2612

As it in Table 4, in the catalyst combination named A11, the slope of the linear relationship of C4 olefin selectivity with temperature was 0.0519. It can be seen that under the catalysis of this catalyst combination, the C4 olefin selectivity is the least sensitive to temperature.

The ethanol conversion ratio and C4 olefin selectivity both increased with the increase of temperature. The ethanol conversion ratio was more sensitive to temperature, while the C4 olefin selectivity was relatively less sensitive to temperature.

3.2. Analyze the Experimental Results of the Same Catalyst Combination at the Same Temperature for Different Experimental Times

According to the data, MATLAB was used to make a line graph corresponding to the selectivity, ethanol conversion ratio and time of each product in the experiment. As it in Figure 2.

With the progress of the reaction time, the ethanol conversion ratio decreased obviously and stabilized after reaching a certain level. The C4 olefin selectivity has a slight fluctuation but no obvious numerical change, which is relatively stable. The selectivity of fatty alcohols with carbon number of 4-12 also decreased significantly, and then stabilized. These two sets of data account for the majority of each product. The selectivities of Ethylene, Acetaldehyde, Methylbenzaldehyde and Methylbenzyl alcohol and other substances were all at low levels and changed little.

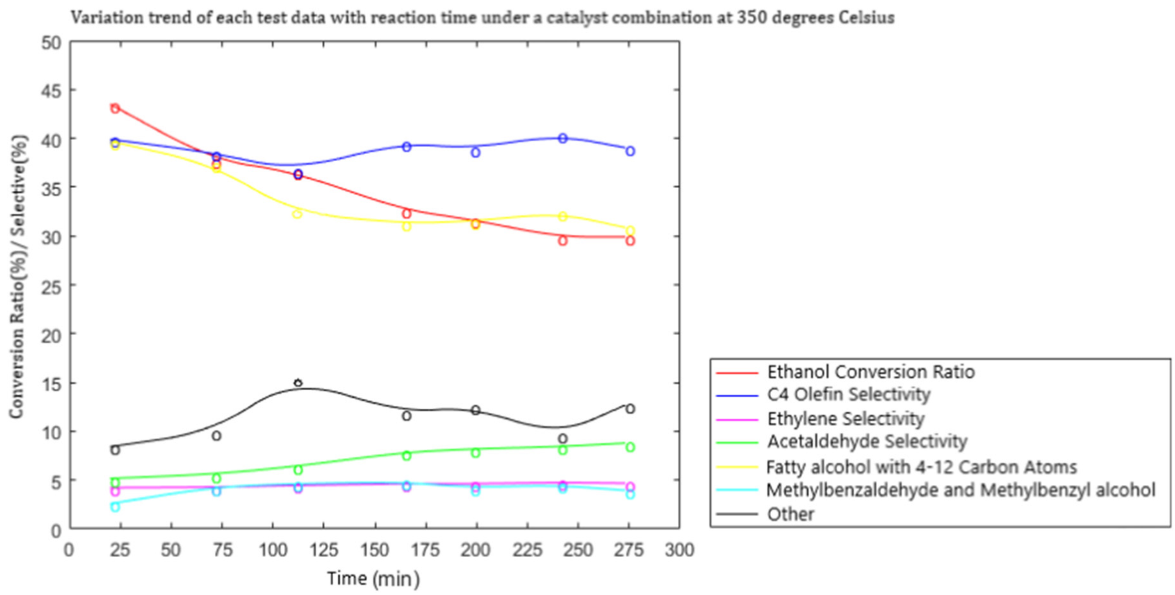


Figure 2. Variation Trend of each Test Data with Reaction Time under a Catalyst Combination at 350 Degrees Celsius

Analyzing the results, it is speculated that the increase in the product accelerates the progress of the reverse reaction, thereby inhibiting the occurrence of the forward reaction.

4. Model Evaluation

4.1. Advantages of the Model

Linear Regression Model: Using linear regression model to analyze the relationship between ethanol conversion ratio, C4 olefin selectivity and temperature, the sensitivity of ethanol conversion ratio and C4 olefin selectivity to temperature can be intuitively obtained by slope. The relationship between ethanol conversion ratio, C4 olefin selectivity and temperature was analyzed accurately.

4.2. Shortcomings of the Model

Linear Regression Model: The fitting degree of the linear equation is slightly inferior to the polynomial, and there may be some errors.

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