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Study on the relationship between temperature and the process of preparing C4 olefin based on ethanol coupling

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Abstract: C4 olefins are widely used in the production of chemical products and pharmaceutical intermediates. Ethanol as a clean energy, the preparation of C4 olefins can protect the environment. Here we mainly study the specific effects of catalyst combination and temperature on the degree of reaction. In this paper, we first draw each group of data on a layer in order to observe the properties of the whole, and then use the mean method to find a curve that can represent the characteristics of the whole. The correlation analysis of the curve is carried out, and then it is known that the effect of temperature on the degree of reaction has a sinusoidal relationship through the reference literature, which is further expressed by mathematical formula. When analyzing the experimental results, we focus on the change of the data, whether it has gone through the extreme value, the relationship between the reaction rate and the formation rate and so on. After the improvement of the model, the thermodynamic formula and kinetic formula were used to study the conversion rate of ethanol and the selectivity of C4 olefins. Finally, it is concluded that the relationship between ethanol conversion and temperature is proportional and has a strong correlation, and the selectivity of C4 olefins is proportional to temperature, but the correlation is moderate; at 350 degrees, the test results of a given catalyst combination at different times of an experiment are analyzed in three aspects.

1. Introduction

In recent years, with the continuous development of new economies such as automobile and chemical industry, the demand for coal and fossil energy is increasing, which leads to a series of problems, such as resource shortage, environmental pollution and so on [1]. Therefore, looking for an alternative renewable energy is the current research hotspot. As a good clean energy, ethanol can be obtained by biomass fermentation such as straw and corn, and its raw materials come from a wide range of sources. With the increase of ethanol production year by year and the decrease of production cost, ethanol as a platform molecule into other value-added products has a broad application prospect. C4 olefin is an important basic chemical raw material. This paper mainly studies the model of preparing C4 olefin by ethanol coupling, and observes the effects of temperature and catalyst on ethylene concentration and C4 olefin selectivity. Finally, the optimal way to prepare C4 olefins was obtained [2].

2. Visual treatment of temperature influence

To facilitate the observation of the overall characteristics, we draw the following image.

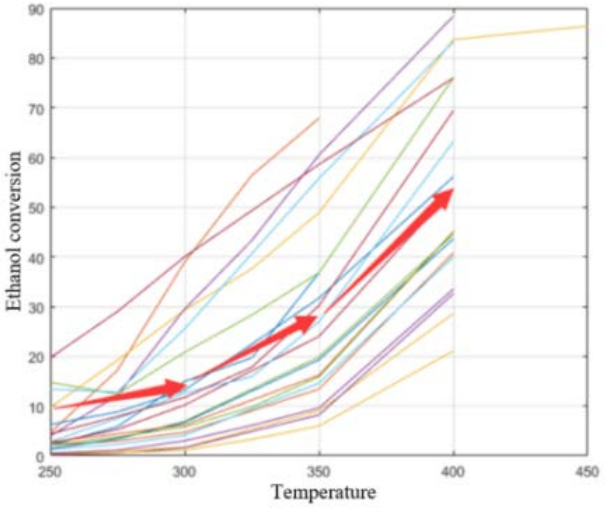

Figure 1: The relationship between temperature and ethanol conversion

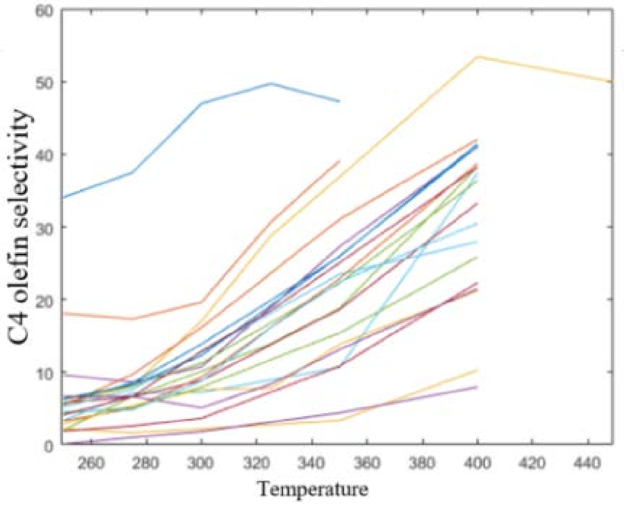

Figure 2: Relationship between temperature and C4 olefins selectivity

When the temperature is in the range of (250,400), the ethanol conversion rate is directly proportional to the temperature. In order to be able to represent all of the samples

3. Correlation Analysis and Test Model Construction

3.1 Averaging treatment

First of all, the averaging process is carried out.

Table 1: Averaging treatment

Temperature	250	275	300	325	350	400
Ethanol conversion	4.6	7.7	13.7	23.8	29.06	53.9
C4 olefin selectivity	6.5	8.2	11.7	20.4	21.8	32.0

3.2 Correlation analysis

The correlation analysis is carried out by using SPSS, and the results are as follows:

Table 2: Correlation coefficient table

					Temperature	Ethanol conversion
Temperature	Pearson correlation.				1	**.954****
	Significant (double tail)					**.003**
	N				6	6
	Repeated sampling c	Deviation			0	.013
		The error of the average			0	.028
		95% confidence interval	Lower limit		1	.899
			Upper limit		1	1.000
Ethanol conversion	Pearson correlation.				.954**	1
	Significant (double tail)				.003	
	N				6	6
	Repeated sampling c	Deviation			.013	0
		The error of the average			.028	0
		95% confidence interval	Lower limit		.899	1
			Upper limit		1.000	1
**. The correlation was significant at 0.01 layer (double tail).						
c. Unless otherwise stated, the results of repeated sampling will be based on 1000 repeated samples						

From the above table, we can see that the Pearson coefficient is 0.954, which has a strong correlation between 0.8 and 1. When the temperature is (250, 400) [3-5], we can approximate the shape by $f(x) = a_1 * \sin(b_1 * x + c_1)$ to describe the relationship between temperature and ethanol conversion, after calculation, we can get the following table:

Table 3: Coefficient table

Coefficient	Value	Confidence interval
a1	16.7	(13.08, 20.31)
b1	0.009329	(0.004149, 0.01451)
c1	4.11	(2.714, 5.506)

Using the same method to analyze the correlation between the selectivity of C4 olefins and temperature, the results are as follows.

Table 4: Correlation coefficient table

					Temperature	C4 olefin selectivity
Temperature	Pearson correlation.				1	**.600**
	Significant (double tail)					**.091**
	N				6	6
	Repeated sampling c	Deviation			0	.003
		The error of the average			0	.311
		95% confidence interval	Lower limit		1	-.091
			Upper limit		1	1.000
C4 olefin selectivity	Pearson correlation.				.600	1.000
	Significant (double tail)				.091	
	N				6	6
	Repeated sampling c	Deviation			.003	0
		The error of the average			.311	0
		95% confidence interval	Lower limit		-0.91	1
			Upper limit		1.000	1
c. Unless otherwise stated, the results of repeated sampling will be based on 1000 repeated samples						

The correlation coefficient is only 0.6000, moderate correlation.

4. Model improvement

Ethanol = ethylene + C4 olefin + acetaldehyde + 4-12 fatty alcohol + methyl + other, in the reaction system, the conversion rate of ethanol can be expressed as follows:

$$X_c = 1\text{-} exp(-M\tau) \tag{1}$$

Where M is the rate coefficient, τ is the residence time of the material, and the rate M generally conforms to the Arrkenius quantity, that is:

$$M = M_0 \, exp(-\frac{Er}{Tr}) \tag{2}$$

Among them, M0 is the frequency factor, Tr is the relative temperature and Er is the apparent activation energy.

$$X_c = 1\text{-} exp(-M_0 \, exp(-\frac{Er}{Tr})\tau) \tag{3}$$

Considering that ethanol is the reactant and C4 olefin is the product in the process of preparing C4 olefin from ethanol, it can be approximately considered that the selectivity of C4 olefin is proportional to the conversion of ethanol, then the fitting function of C4 olefin selectivity is as follows:

$$C_4 = \widetilde{M}(1 - exp(-b \, exp(-\frac{a}{T}))) \tag{4}$$

5. Model analysis

(a) The conversion rate of ethanol is decreasing continuously, whether it has passed the maximum value or not.

First of all, for the reasons for the continuous decline of ethanol conversion: at 350 degrees, the ethanol conversion should be 15.4%, while when 20min, the ethanol conversion should be 43.5, there are two cases:

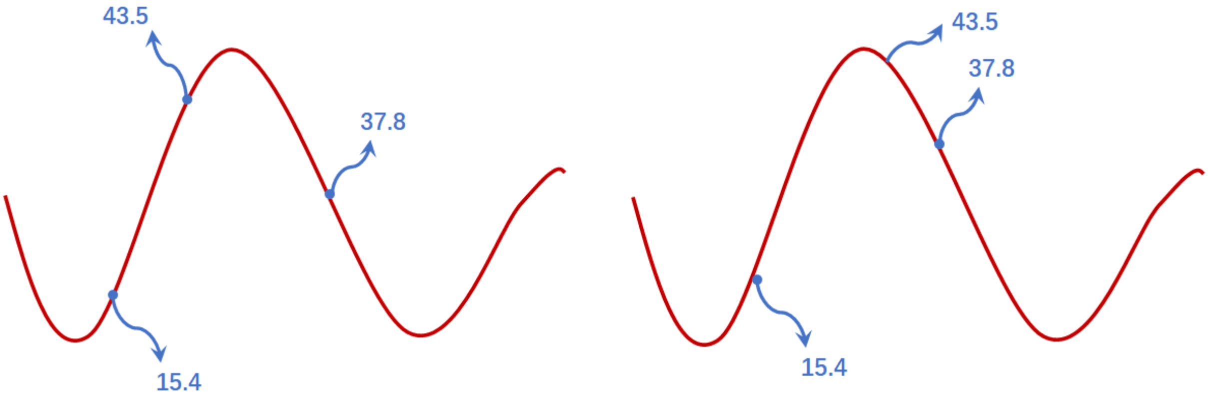

Figure 3: Schematic diagram of continuous decrease in ethanol conversion

(b) The change range of C4 olefin selectivity is small.

C4 olefins are products, and other products are formed in the process of reaction.

We note that at 350 degrees, some of the olefin selectivity is as follows:

Table 5: Olefin selectivity results

Catalyst combination number	Ethanol conversion (%)
A3	2.85
A9	2.84
A2	2.76
A13	2.53
A7	2.28
A4	2.23
B2	2.11

The catalyst can increase the reaction rate. In the case of the same temperature and different catalyst combinations, the change of ethanol conversion degree is small, which means that in the process of reaction, when the amount of ethanol reaches a certain value, it will begin to produce other products. At the same time, the relationship between the selectivity of C4 olefins and the degree of ethanol conversion was analyzed.

C4 olefin is a product and ethanol is a reactant, which is approximately proportional to each other.

6. Conclusion

In this paper, a curve which can represent the overall characteristics is obtained by using the mean method, and then the correlation analysis is carried out and further expressed by mathematical formula. Then it focuses on the analysis of the change of the data, whether it has passed the extreme value, the relationship between the reaction rate and the formation rate and so on. After the improvement of the model, the thermodynamic formula and kinetic formula were used to study the conversion rate of ethanol and the selectivity of C4 olefins. Finally, it is concluded that the relationship between ethanol conversion and temperature is proportional and has a strong correlation, and the selectivity of C4 olefins is proportional to temperature, but the correlation is moderate; at 350 degrees, the test results of a given catalyst combination at different times of an experiment are analyzed in three aspects.

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