# Study on preparation of Olefins by Coupling ethanol based on simulated annealing Model and Neural Network algorithm

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**Abstract.** Ethanol molecules can be prepared by biomass fermentation, with a wide range of sources, green and clean, and the production of high value-added C4 alkenes with ethanol as a platform molecule has great application prospects and economic benefits has attracted wide attention at home and abroad. Meanwhile, optimizing the reaction conditions for the preparation of butene can also appropriately reduce the waste of resources and make a certain contribution to environmental protection. This paper collects relevant response data, uses fit type and Linear model for data fitting and comparative analysis, calculates the average value of each item of data selected from the five experimental groups, and then uses MATLAB two-dimensional broken line drawing for analyzing the changing law of the data more vividly and intuitively. Finally, the simulated annealing algorithm model and the genetic algorithm model are used to optimize the temperature and catalyst combination of the highest C4 olefin yield, the GRGNon-Linear method, the simple simplex method, and the Evolutionary evolution algorithm and Nesterovmethod artificial firefly algorithm are used to analyze and calculate. Thus, the optimal catalyst combination is 200mg1wt%Co/SiO2-200mgHAP ethanol concentration 0.9ml/min, and the temperature of 425℃ is the maximum yield of C4 olefins. Moreover, 350 degrees is the optimum temperature in the temperature range below 350 degrees. Finally, we use the experimental data of the BP (BackPropagation) neural network prediction algorithm to predict and analyze the feasible scheme and explain the detailed reasons for choosing the experimental conditions to determine five groups of better experimental schemes.

**Keywords:** Component; formatting; style; styling; insert.

## 1. Introduction

Butene is one of the important basic chemical raw materials, which is widely used in chemical products and pharmaceutical intermediates [1]. Meanwhile, butene is the raw material for synthesizing SEC butanol and dehydrogenation to butadiene. CIS and trans isomers of 2-butene are used to synthesize C4 and C5 derivatives and prepare superimposed gasoline and the crosslinking agent. Isobutylene is the raw material for manufacturing butyl rubber and polyisobutylene rubber. It can also react with formaldehyde to produce isoprene, which is used to make polyisobutylene polymers with different molecular weights, and it can be used as lubricating oil additives and resins through processing. Traditional production methods will use fossil energy as raw materials [2]. With the continuous deepening of national energy conservation and emission reduction policies, the development of new clean energy is becoming more and more urgent. Moreover, ethanol molecules can be prepared by corn slurry fermentation. It has a wide range of sources and is green. Using it as a platform molecule to produce high value-added C4 ene has great application prospects and can bring considerable economic benefits. Therefore, it has attracted extensive attention at home and abroad.

Different combinations of catalysts will affect the conversion of ethanol and the selectivity of C4 olefins, and the catalytic effect will also be affected by external temperature [3]. It will affect the efficiency of preparing C4 olefins and increase the plant's time cost and purification cost. In order to improve the comprehensive efficiency and reduce the waste of resources, we need to explore the process conditions for the preparation of C4 olefins by ethanol catalytic coupling and comprehensively obtain the best reaction conditions to maximize the comprehensive benefits of the whole process. Ethanol is the raw material for the preparation of C4 olefins. In the process of

preparation, the catalyst combination and temperature used in the reaction has an effect on the selectivity and yield of C4 olefins. In order to improve the comprehensive efficiency and reduce the waste of resources, we need to explore the process conditions for the preparation [4-6] of C4 olefins by ethanol catalytic coupling and comprehensively obtain the best reaction conditions in order to maximize the comprehensive benefits of the whole process. This paper focuses on the modeling and analysis of this process.

## 2. Mean value Analysis and selective judgment

Select the following five experimental groups with high ethanol conversion rate and high selectivity of C4 olefins for analysis, and solve the mean value of each group's data [7]. The specific screening and calculation results are shown in the table below (the data in the table are the mean value, and four decimal places are reserved)

**Table 1.** Specific screening and calculation results 01

| Catalyst combination number | Catalyst combination | Ethanol conversion (%) | Ethylene selectivity (%) | C4 olefin selectivity (%) |
|---|---|---|---|---|
| A3 | 200mg 1wt%Co/SiO2200mg HAP- ethanol concentration 0.9ml/min | 44.9714 | 3.9214 | 28.4928 |
| A4 | 200mg 0.5wt%Co/SiO2200mg HAP- ethanol concentration 1.68ml/min | 39.6333 | 1.3483 | 19.3533 |
| A6 | 200mg 5wt%Co/SiO2200mg HAP- ethanol concentration 1.68ml/min | 38.1600 | 4.5420 | 13.1120 |
| B6 | 75mg 1wt%Co/SiO275mg HAP- ethanol concentration 1.68ml/min | 21.500 | 1.1700 | 14.5016 |
| B7 | 100mg 1wt%Co/SiO2100mg HAP- ethanol concentration 0.9ml/min | 23.5666 | 0.9900 | 17.5383 |

**Table 2.** Specific screening and calculation results 01

| Catalyst combination number | Acetaldehyde selectivity (%) | Selectivity of fatty alcohol with a carbon number of 4-12 (%) | Selectivity of methyl benzaldehyde and methyl benzyl alcohol (%) | Selectivity of other products(%) |
|---|---|---|---|---|
| A3 | 5.2657 | 49.8428 | 3.2071 | 9.2700 |
| A4 | 4.6000 | 59.7316 | 7.4116 | 7.5550 |
| A6 | 25.1200 | 45.2620 | 3.3060 | 8.8580 |
| B6 | 6.2416 | 69.6716 | 4.9400 | 8.4750 |
| B7 | 7.4416 | 61.4900 | 5.8867 | 6.7283 |

Then, through MATLAB drawing, the two-dimensional broken line diagram is used to more vividly and intuitively analyze the change law of data. The drawn image is as follows

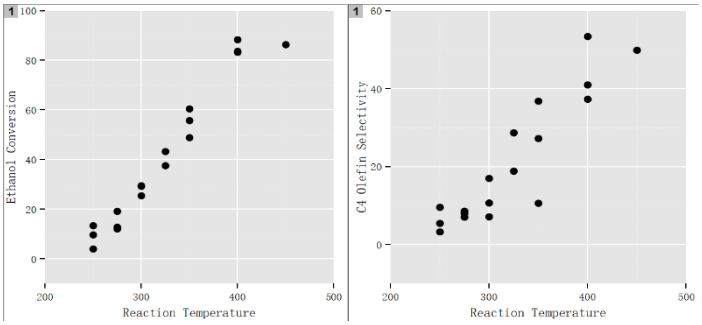


**Figure 1.** Selectivity of data in A

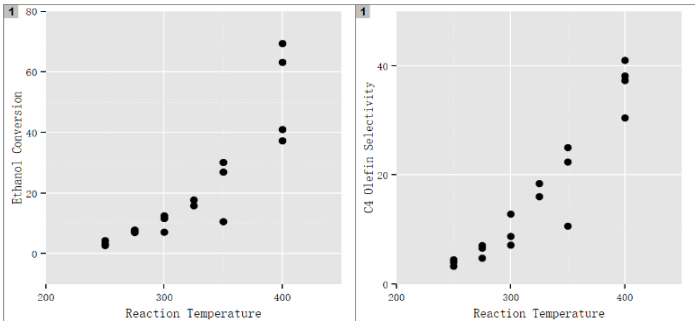


**Figure 2.** Selectivity of data in B

By analyzing the above tables and images, we can know that the reaction temperature can be appropriately increased but not too high. At this appropriate temperature, the conversion of ethanol and the selectivity of C4 olefins can be increased, and the selectivity of other by-products can be reduced. According to the analysis results, the catalyst combination of group A3 is 200mg1wt% Co / sio2-200mghap, and the ethanol concentration is 0.5%. When the reaction temperature was 400 ℃, the maximum conversion rate of ethanol was 83.9 ml/min and 7133815760754%. The highest selectivity of C4 olefins is 53.5% 43%, and the selectivity of other by-products was lower than that of other experimental groups; Furthermore, the catalyst combination of group A4 is 200mg0 5wt% Co / sio2-200mg HAP ethanol concentration 1 68ml/min, when the reaction temperature is 400 ℃, the maximum conversion rate of ethanol is 88 4%, C4 olefin has the highest selectivity, with a value of 41.5% The selectivity of other by-products was lower than that of other experimental groups. However, the average ethanol conversion rate of group A3 is higher than that of group A4, so the conditions set by group A3 are the most suitable for the organic reaction.

Moreover, the longer the reaction time of the organic reaction, although the conversion of ethanol will be reduced, the selectivity of C4 olefins will increase, and the selectivity of other by-products will be appropriately reduced. It is necessary to consider an appropriate scheme to maximize the conversion of ethanol and the selectivity of C4 olefins. To sum up, the catalyst combination is 200 mg 1wt% Co / sio2-200 mg HAP ethanol with a concentration of 0.5% 9ml / min, the reaction temperature is 400 degrees, and the reaction time is 240Min, which is the ideal reaction state that can be predicted. Recently, the catalyst combination. The higher the fitting degree between the reaction temperature and time and the above experimental group, the greatest benefit will be brought.

## 3. Optimal conversion rate model

We use the GRGNon-Linear method, a common method to solve nonlinear programming. Most of the time, according to the change of input value (variable) and the change rate of the objective function, we judge whether to get a local optimal solution or not and use the Simplex simplex method to solve it. Finally, we use the Evolutionary evolution algorithm and Nesterov method artificial firefly algorithm to construct and solve the optimal solution of the problem. Through the characteristics of the catalyst, it is known that its activity, related spatial structure, and unit cell structure will be affected by temperature. It is analyzed by the GRGNon-Linear method. It can be concluded that the

temperature will affect the conversion of ethanol and the selectivity of C4 olefins and further affect the above two dependent variables by affecting the relevant properties of the catalyst. Then the Simplex simplex method, evolutionary evolution algorithm, and Nesterov method artificial firefly algorithm are used, so we take the temperature of the reaction time as the main influencing factor.

### 3.1. Modeling process

The specific process is as follows:

(1) Initialization: initial temperature T (large enough), initial solution state s (the starting point of algorithm iteration), and the number of iterations of each t value L;

(2) Steps (3) to (6) for k = 1,..., l;

(3) Generate a new solution s';

(4) Calculation increment Δ T ′ = C (s ′) - C (s), where C (s) is the evaluation function;

(5) If Δ If t ′ < 0, accept s ′ as the new current solution, otherwise take the probability as exp (- Δ T '/ T) accept s' as the new current solution;

(6) If the termination conditions are met, the current solution is output as the optimal solution to end the program; The termination condition is usually taken as that the algorithm is terminated when several new solutions in succession are not accepted;

(7) T decreases gradually and T - > 0. In the final Matlab drawing research, the image is as follows:

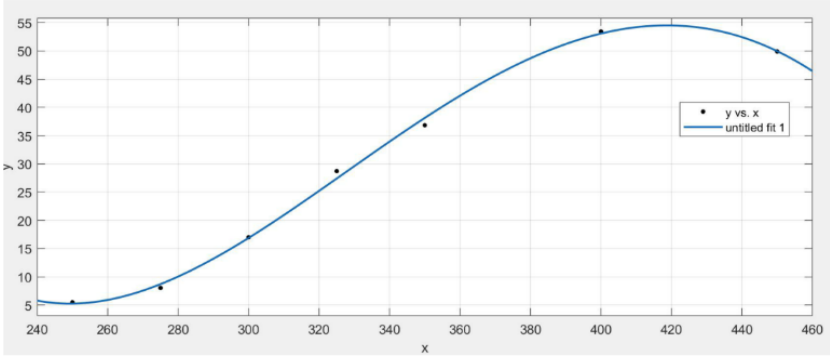


**Figure 3.** Fourth power optimal temperature prediction diagram

The results are as follows:

$$
\begin{aligned}
&f(x) = p_1 \times x^4 + p_2 \times x^3 + p_3 \times x^2 + p_4 \times x + p_5 \\
&p_1 = 2.801\text{e}^{-8}\ (-2.226\text{e}^{-7},\ 2.787\text{e}^{-7}) \\
&p_2 = -5.767\text{e}^{-5}\ (-0.0004073,\ 0.000292) \\
&p_3 = 0.03864\ (-0.1418,\ 0.2191) \\
&p_4 = -10.25\ (-51.06,\ 30.57) \\
&p_5 = 943.7\ (-2471,\ 4358)
\end{aligned}
\tag{1}
$$

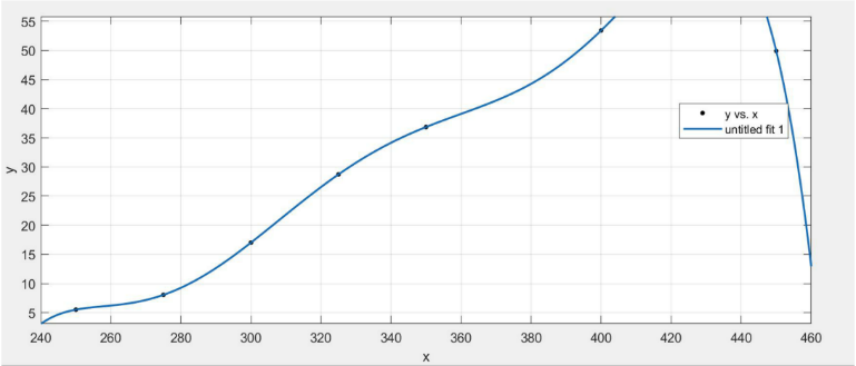


**Figure 4.** Sixth power optimal temperature prediction diagram

$$
\begin{aligned}
&f(x) = p_1 \times x^6 + p_2 \times x^5 + p_3 \times x^4 + p_4 \times x^3 \\
&+ p_5 \times x^2 + p_6 \times x + p_7 \\
&p_1 = \text{-}6.922\text{e}^{\text{-}11} \\
&p_2 = 1.386\text{e}^{\text{-}7} \\
&p_3 = \text{-}0.0001145 \\
&p_4 = 0.04992 \\
&p_5 = \text{-}12.12 \\
&p_6 = 1554 \\
&p_7 = -8.221e^{-4}
\end{aligned} \tag{2}
$$

Based on the analysis of the optimal conditions of the organic reaction, the catalyst combination of group A3 in the experimental group is the combination to obtain the optimal state of C4olefin yield (200mg1wt%Co/SiO2-200mg HAP-ethanol concentration 0.9ml/min) and the above prediction of the optimal reaction temperature by simulated annealing algorithm model. The temperature condition of 425C is about the temperature value of the maximum C4olefin yield. If the temperature is lower than 350 degrees, it can be seen that the yield of C4 olefins increases with the increase of temperature in this range, so the maximum temperature value of the yield of C4 olefins below 350 degrees is 325 degrees.

## 4. Combination Analysis of Catalysts based on Neural Network

Based on the above various reaction conditions for the organic reaction and different combinations of catalysts, the selectivity of reactant ethanol and C4 olefins, and other by-products are different. According to the analysis, the specific experimental scheme is shown in the following table:

**Table 3.** Specific experimental scheme

| Experimental group | Catalyst combination | Reaction temperature | Reaction time |
|---|---|---|---|
| 1 | 200mg 1wt% Co/SiO2-200mg HAP- ethanol concentration 0.9ml/min | 375 | 240 |
| 2 | 200mg 1wt% Co/SiO2-200mg HAP- ethanol concentration 0.9ml/min | 425 | 240 |
| 3 | 200mg 1wt% Co/SiO2-200mg HAP- ethanol concentration 0.9ml/min | 475 | 240 |
| 4 | 200mg 1wt% Co/SiO2-200mg HAP- ethanol concentration 0.9ml/min | 425 | 240 |
| 5 | 200mg 1wt% Co/SiO2-200mg HAP- ethanol concentration 0.9ml/min | 450 | 240 |

According to the analysis of the control group's results under different conditions, the experimental group A4 had the highest conversion of ethanol (the catalyst combination was 200mg0.5wt%Co/SiO2-200mgHAP-ethanol concentration 1.68ml/min, and the reaction temperature was 400C). At this time, the conversion of ethanol was the highest among the 21 experimental groups. With the increase of temperature, the selectivity of C4 olefins in the experimental group also increased and showed an upward trend in the experimental range of 400 degrees. Therefore, we chose two experimental groups with an increase of 425C and 450C under this condition to explore whether the selectivity of C4 olefins will continue to increase with the increase of temperature in the case of catalyst combination 200mg0.5wt%Co/SiO2-200mgHAP-ethanol concentration 1.68ml/min. At the same time, among the 21 experimental groups, the experimental group A3 had the highest selectivity

for C4 olefins (the catalyst combination was 200mg1wt%Co/SiO2-200mgHAP-ethanol concentration 0.9ml/min, and the reaction temperature was 400C). At this time, the conversion of ethanol was not much different from the highest ethanol conversion of 400 degrees in the A4 group. However, with the temperature increase in this experimental group, the ethanol conversion and the selectivity of C4 olefins increased from 250 degrees to 400 degrees. However, in the process, from 400 degrees to 450 degrees, the ethanol conversion increased, and the selectivity of C4 olefins decreased. By reducing the experimental temperature range, we explore whether there is a temperature that can make the selectivity of C4 olefins higher than 400C when the catalyst combination is 200mg1wt%Co/SiO2-200mg HAP-ethanol concentration 0.9ml/min. Therefore, we set three different temperature experimental groups under this condition, namely, 375C, 425C, 475C.

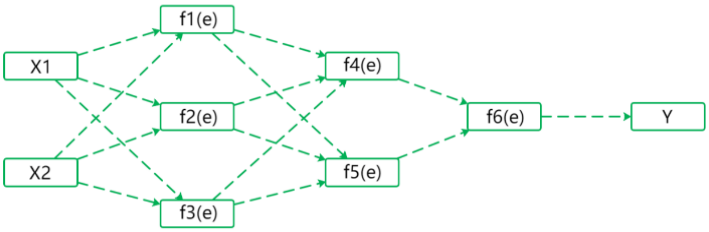


**Figure 5.** Neural network flow

The rate increases, and the selectivity of C4 olefins decreases. By reducing the experimental temperature range, we explore that when the catalyst combination is 200mg1wt% Co / sio2-200mghap, ethanol concentration is 0. In the case of 9ml / min, whether a temperature before and after 400 degrees can make the selectivity of C4 olefins higher than 400 degrees, we set three different temperature experimental groups under this condition 375 degrees, 425 degrees, and 475 degrees.

We conduct specific data analysis, where X represents the data of the input layer, followed by F representing various relevant influencing factors of the data contained in the hidden layer, and finally, summarize each data to output more accurate data y to achieve a more accurate purpose.

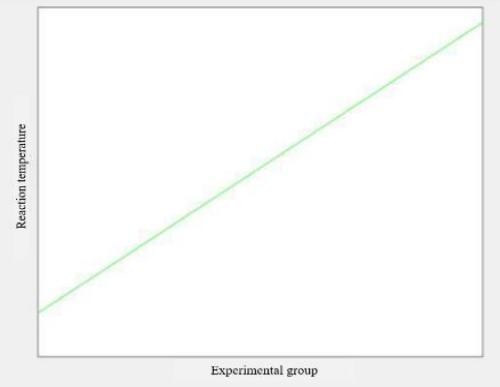


**Figure 6.** First set of catalyst combination data

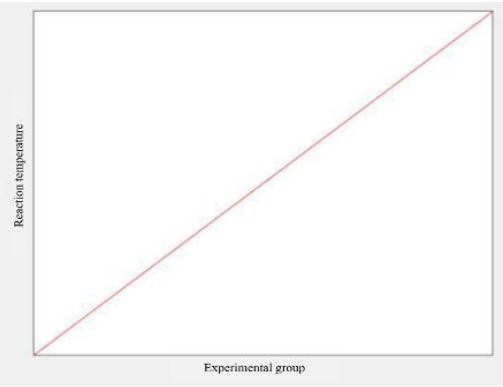


**Figure 7.** Second set of catalyst combination data

## 5. Conclusions

As one of China's most important basic chemical raw materials, butene is widely used in chemical products and pharmaceutical intermediates. Its traditional production methods use fossil energy as raw materials. with the change of the natural environment and the continuous deepening of national energy conservation and emission reduction policies, it is more and more urgent to develop new types of clean energy. Ethanol molecules can be prepared by biomass fermentation, with a wide range of sources, green and clean, and the production of high value-added C4 olefins with ethanol as a platform molecule has great application prospects and economic benefits has attracted wide attention at home and abroad. Therefore, in this paper, the average values of the data of the five experimental groups are calculated, and then the changing rules of the data are analyzed more visually through the two-dimensional broken line drawing of MATLAB. It is concluded that the catalyst combination is 200mg1wt%Co/SiO2-200mg HAP-ethanol concentration 0.9ml/min, and the reaction temperature is 400C and the reaction time is 240min. The best reaction state can be predicted at present. The higher the reaction temperature and time and the degree of fit between the catalyst combination and the above experimental group, the greater the conversion of ethanol and the selectivity of C4 olefin. Then the simulated annealing algorithm model and the genetic algorithm model are used to optimize the temperature and catalyst combination of the highest C4 olefin yield, the GRGNon-Linear method, the simple simplex method, and the Evolutionary evolution algorithm and Nesterovmethod artificial firefly algorithm are used to analyze and calculate. Thus, the optimal catalyst combination is 200mg1wt%Co/SiO2-200mgHAP ethanol concentration 0.9ml/min, and the temperature of 425 ℃ is the maximum yield of C4 olefins. Moreover, 350 degrees is the optimum temperature in the temperature range below 350 degrees. Finally, we use the experimental data of the BP (BackPropagation) neural network prediction algorithm to predict and analyze the feasible scheme and explain the detailed reasons for choosing the experimental conditions to determine five groups of better experimental schemes.

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