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BP-Based Model of Influence of Ethanol Catalyst Combination on C4 Yield.

Haomiao Niu[1,2], Xianghao Hu[2], Caiyue Yuan[2]

1. North China University of Science and Technology Mathematical Modeling Innovation Lab, Tangshan 063210, China.

2. College of Chemical Engineering, North China University of Science and Technology, Tangshan 063210, China.

Abstract: In this paper, aiming at the influence of catalyst combination and temperature in the experiment of preparing C4 olefins by ethanol coupling, according to the different requirements of the experiment, the functional relationship between ethanol conversion rate, C4 olefin selectivity and temperature was obtained by polynomial fitting. Secondly, following the principle of controlled variables, the optimal process conditions for preparing C4 olefins by ethanol coupling were designed through the chemical synthesis model based on BP neural network.

Keywords: Polynomial Fitting; BP Neural Network; Principle of Controlling Variables.

1. Question background

The questions come from Question B of the National Mathematical Modeling Competition for College Students in 2021. According to the experimental data obtained in Appendix 1 and Appendix 2, the following questions are completed through mathematical modeling:

(1) analyze each catalyst combination in annex 1, and study the relationship between ethanol conversion rate, C4 olefin selectivity and temperature.

(2) The effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity were discussed.

(3) Select the optimum catalyst combination and temperature, so as to make the C4 olefin yield as much as possible under the same experimental conditions.

High. When the temperature is lower than 350℃, the optimum catalyst combination and temperature are selected to make the C4 olefin yield as high as possible.

2. Problem Analysis

In essence, the problem of preparing C4 olefins by ethanol coupling is to explore the effects of different catalyst combinations and temperatures on the preparation of olefins (ethanol conversion, C4 olefin selectivity and C4 olefin yield), find out the relationship between catalyst combinations and temperatures and various preparation effects, and explore the technological conditions for preparing C4 olefins by ethanol coupling, thus providing data support for people to carry out experiments under different environmental conditions.

3. Model Assumptions

The data obtained by laboratory experiments have good reliability and typicality. The error between the actual catalyst combination and the recorded catalyst combination caused by operation error and calculation error during the experiment is not considered.

4. Establishment and solution of the model.

4.1 The establishment and solution of problem one model.

4.1.1 Establishment of Model for Question

Based on the data of each catalyst combination in Annex I, the relationship between ethanol conversion rate, C4 olefin selectivity and temperature was studied. Taking temperature as independent variable X and ethanol conversion rate and C4 olefin selectivity as dependent variable Y, the data were fitted by polynomial [1].

4.1.2 Solution of Problem One Model.

1) Relationship between ethanol conversion rate and temperature.

The first, second and third polynomial fitting of temperature to ethanol conversion rate is carried out respectively, because there are too few catalyst data in each group, only five different temperatures and too few training sets, and the over-fitting phenomenon is caused by high-order fitting. The first-order polynomial fitting is lower than the second-order polynomial fitting, so the second-order polynomial fitting is chosen to describe the relationship between ethanol conversion rate (y_i) and temperature (x_i). The fitting equation is:

$$p_2(x) = a_0 + a_1 x + a_2 x^2 \quad (1)$$

Table of coefficients a0, a1 and a2 in different catalyst combinations:

Table 1 Quadratic fitting parameter diagram of ethanol conversion rate and temperature

serial number	a_0	a_1	a_2
A1	141.7531	-1.1935	0.0025
A2	-227.3925	1.1057	-0.0007
		……	
B1	121.2379	-0.9484	0.0019
B2	188.2547	-1.3647	0.0025

Similarly, the relationship between C4 olefin selectivity and temperature can be obtained, which is not shown here.

4.2 The establishment and solution of problem 2 model

The effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity were studied. The effects of different catalyst combinations (i.e., the combination of Co loading, Co/SiO_2 and HAP loading ratio, and ethanol concentration) on ethanol conversion and C4 olefin selectivity were studied by using the control variable method.[2].

4.2.1 BP neural network model based on simulation experiments of different temperatures and catalyst combinations

1) BP neural network model

By observing the data characteristics in Annex 1, 21 groups of different catalyst combinations at temperatures of 250℃, 275℃, 300℃ and 350℃ were selected, and a total of 84 sample data were used as the input data of the model. Among them, 70% data is used as training set, 15% data as verification set, and 15% data as test set. There are 8 hidden neurons and 2 output layers.[3,4].

The trained network is used to simulate the original data, and the difference between the simulation value and 84 sample data is obtained to obtain the difference distribution diagram between the model result and the sample.

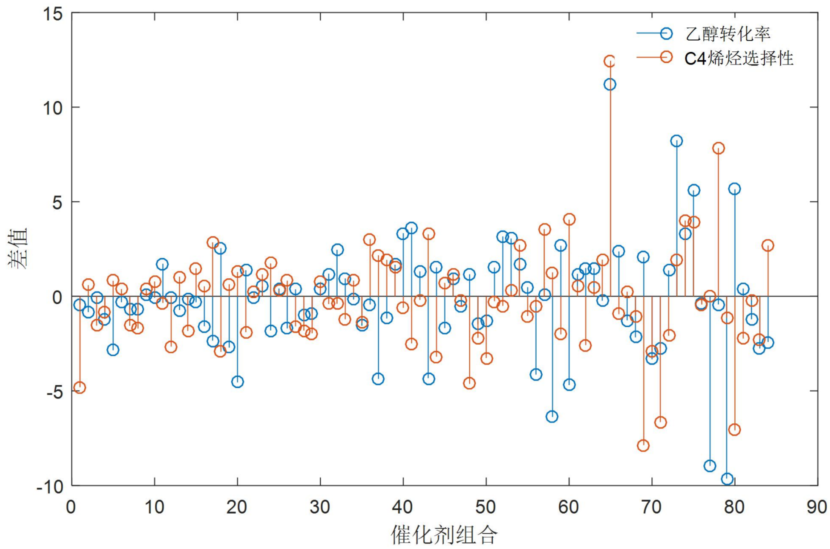

Fig. 1 Distribution of difference between model results and samples

The catalyst combinations in which the absolute value of the difference between the simulated value and the sample data is greater than 5 are shown in the following table:

Table 2 Combination table of temperature and catalyst with large error

Catalyst combination	Co/SiO_2 HAP Charging ratio	Co/SiO_2 quality （mg）	HAP quality （mg）	Co load （wt%）	Ethanol concentration （ml/min）	temperature （℃）
B5	1.00	50	50	1	2.1	250
B6	1.00	75	75	1	1.68	350
			……			
A6	1.00	200	200	5	1.68	275
A6	1.00	200	200	5	1.68	300

2）The result and analysis of BP neural network model.

Combined with the model simulation results and the preliminary analysis of the attachment data in question 2, the conclusions in different catalyst combinations and temperatures are drawn:

1、The order of influence on ethanol conversion is temperature > Co loading > Co/SiO_2 and HAP loading ratio > ethanol concentration > HAP mass =Co mass.

2、The order of selectivity to C4 olefins is temperature > ethanol concentration > charge ratio of Co/SiO_2 and HAP > Co loading > HAP mass =Co mass.

4.3 Problem 3 model establishment and solution

4.3.1 Model establishment

On the basis of solving the second problem, according to the attached data and following the principle of single variable, in the catalyst combinations: the charging ratio of Co/SiO_2 and HAP, the mass of Co/SiO_2, the mass of HAP, the load of Co and the concentration of ethanol, only one variable is changed at a time to obtain 14 different catalyst combinations, and 98 groups of sample data are obtained by setting 7 temperature gradients at the same time. Some data are shown in the following table:

Table 3 Table of different catalyst combinations at different temperatures

Co/SiO_2 and HAP charge ratio	Co/SiO_2 quality (mg)	HAP quality (mg)	Co load (1wt%)	Ethanol concentration (ml/min)	temperature (℃)
0.5	33	67	0.5	0.3	275
0.5	33	67	0.5	0.3	300
		……			
1	200	200	5	2.1	100
1	200	200	5	2.1	425

Using the network structure trained by the neural network model in question 2, the ethanol conversion rate and C4 olefin selectivity of 98 groups of sample data were obtained by experimental simulation.

Calculate C4 olefin yield by formula:

$$\text{C4 olefin yield} = \text{Ethanol conversion} \times \text{C4 olefin selectivity} \quad (2)$$

4.3.2 Analysis of model results

Using the network obtained by neural network in question 2, 98 C4 olefin yields were obtained by experimental simulation of 98 sample data, as shown in the figure:

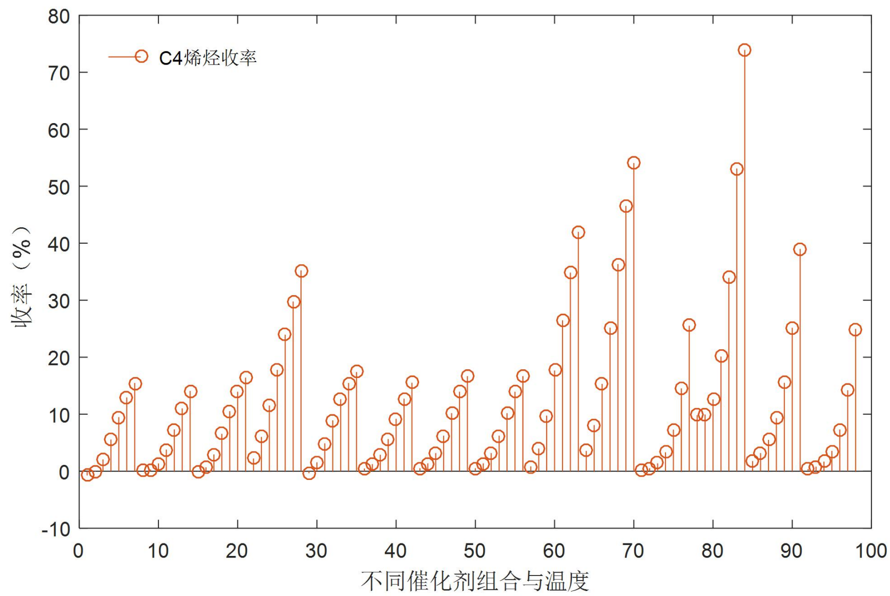

Fig. 2 Needle diagram of C4 olefin yield distribution

As shown in the above figure, it is concluded that:

1. when the catalyst combination is the same, the yield of C4 olefins gradually increases with the increase of temperature;

2. At the same temperature, the yields of C4 olefins are different with different catalyst combinations.

Among the 14 groups of catalyst combinations, the sample data of each group at the highest C4 olefin yield was selected, and a total of 14 groups of data were observed, and the conclusion could be drawn: among the 14 groups of catalyst combinations, the C4 olefin yield was the highest at the temperature of 425℃; The yield of C4 olefin is up to 73.90%, the catalyst combination is 200mg 1wt%Co/SiO_2-200mg HAP- ethanol concentration is 2.1ml/min, and the temperature is 425℃.

Similarly, in the sample data, when the temperature is lower than 350℃, the best catalyst combination is:

200mg 2wt%Co/SiO_2-200mg HAP- ethanol concentration 1.68ml/min, temperature 325℃, the yield of C4 olefin is 15.32%.

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