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Quantification of C4 Olefin Yield based on BP Neural Network and 0-1 Planning Model

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Abstract

With the continuous development of the chemical industry, C4 olefins play an increasingly widespread role in the production of pharmaceuticals and products. In the preparation of C4 olefins, temperature affects the selectivity and ethanol conversion of C4 olefins to varying degrees, which in turn affects the yield of C4 olefins. In this paper, we investigate and analyze the effects of different catalyst combinations and temperatures on the selectivity and ethanol conversion of C4 olefins based on the relationship between the data of each index and time for a given temperature and catalyst combination, and calculate the catalyst combination and temperature that maximize the yield of C4 olefins. The catalyst combination and temperature that maximizes the yield of C4 olefins below 350°C were calculated.

Keywords

Contrast Analysis; BP Neural Network; 0-1 Planning; Quantitative Study.

1. Introduction

Olefins are mainly derived from petroleum and are intermediates of pharmaceuticals as well as important raw materials for the petrochemical industry. However, with the rising energy demand and sharp shortage of fossil energy, it is a trend to find alternative methods to petroleum to prepare olefins and to develop new clean energy sources. Ethanol has received widespread attention as a cheap and easily available, green and clean energy source, and the production of C4 olefins from ethanol is expected to be the main method for the preparation of olefins in the future. In this experiment we investigate the effect of catalyst and temperature on the conversion of ethanol and the selectivity of C4 olefins, which is of great significance for our future focus on the development of ethanol coupling for the preparation of C4 olefins.

The relationship between C4 olefin selectivity and ethanol conversion versus temperature was determined for each catalyst combination fixed. The effects of different catalyst combinations and temperatures on C4 olefin selectivity and ethanol conversion were analyzed. We combined four variables under each catalyst combination with the reaction temperature to obtain a quantifiable set of independent variables, and then visualized the relationship between the categorical variables by SPSS starting from the preparation of cross-tabulations. The relationships between C4 olefin selectivity and ethanol conversion with catalyst combinations and temperature, respectively, were also qualitatively analyzed by the simple control variables method, and it was decided to construct a BP neural network model with the number of nodes in the input layer as 5 and the number of nodes in the output layer as 2.

And based on this, the catalyst combination and temperature that makes the maximum C4 olefin yield are explored, and all possible index values are combined, so the 0-1 planning model is used. The temperature gradient was also set to 5 degrees Celsius in order to seek the possibility of high C4 olefin yield for more combinations. This model can also be used to derive the catalyst combination and

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temperature with the highest C4 olefin yield below 350°C by changing the upper and lower temperature constraints.

2. BP Neural Network Model Construction and Solution

2.1 Model Analysis

In this chapter, we use SPSS to analyze the relationship between categorical variables visually by transforming the frequencies in the cross-tabulations with the idea of dimensionality reduction[1]. After importing the basic data into SPSS, we can get the discriminant measure graph and the multiple correspondence analysis graph, as shown in Figure 1 and Figure 1.

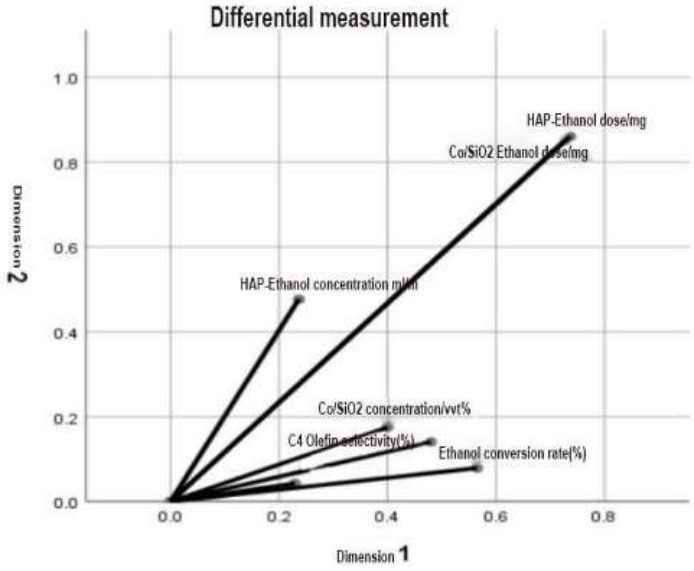

Figure 1. Discriminative metric chart

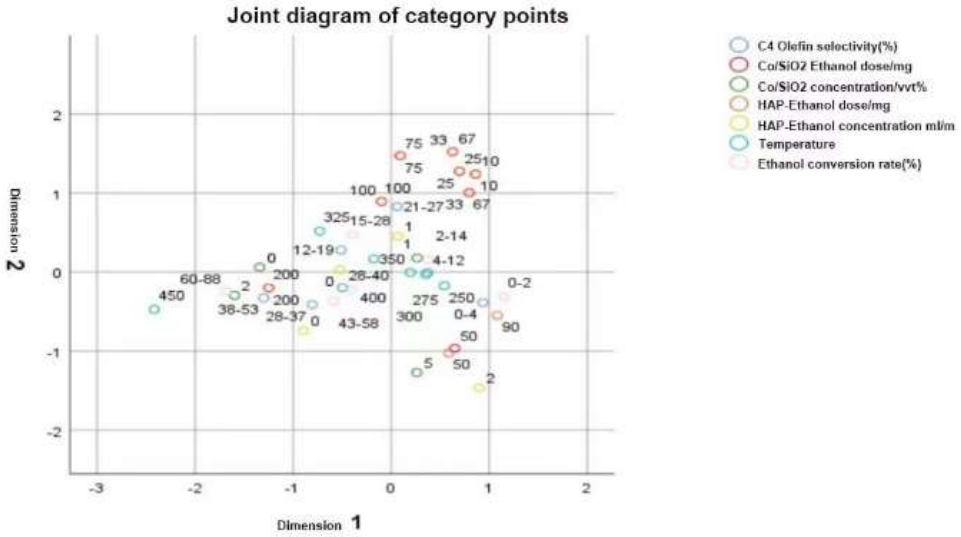

Figure 2. Multiple correspondence analysis chart

The positions of the scattered points in the discriminant measure diagram reflect the degree of differentiation of each variable in two dimensions. Multiple correspondence analysis diagrams are analyzed from the origin (0,0), where different categories of the same variable close to the same orientation and in the same region are similar in nature; different categories of the same variable in

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the same orientation and in the same region may be related to each other. Here, the composition of the catalyst belongs to different categories of the same variable, and the conversion of ethanol and the selectivity of C4 belong to different categories of the same variable, while the composition of the catalyst, time and the conversion of ethanol and the selectivity of C4 belong to different variables. From the multivariate analysis, it can be seen that the ethanol conversion is in the same region as temperature, HAP-ethanol dose, and C4 olefin; the C4 olefin selectivity is in the same region as temperature, HAP-ethanol dose, and ethanol conversion. It can be concluded from the analysis that there may be a direct relationship between the temperature and the HAP-ethanol dose in the catalyst and the ethanol conversion and C4 olefin selectivity.

2.2 Qualitative Analysis of C4 Olefin Selectivity and Ethanol Conversion as a Function of Catalyst Combination and Temperature, Respectively

We made three-dimensional coordinate plots of C4 olefin selectivity versus Co/SiO2 dose and Co loading (as in Figure 3), and C4 olefin selectivity versus HAP dose and ethanol concentration (as in Figure 4), respectively.

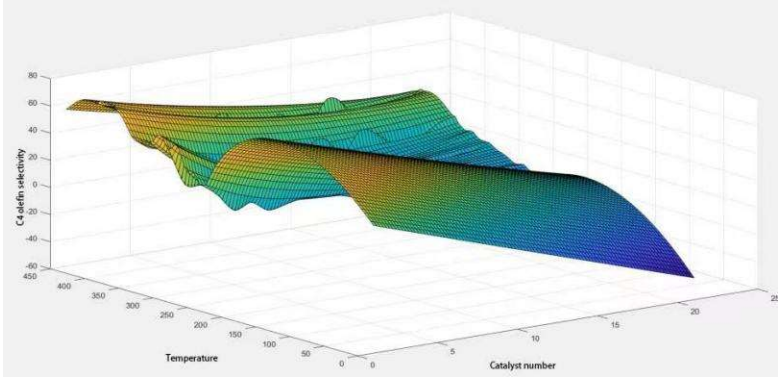

Figure 3. C4 olefin selectivity versus Co/SiO2 dose and Co loading in 3D

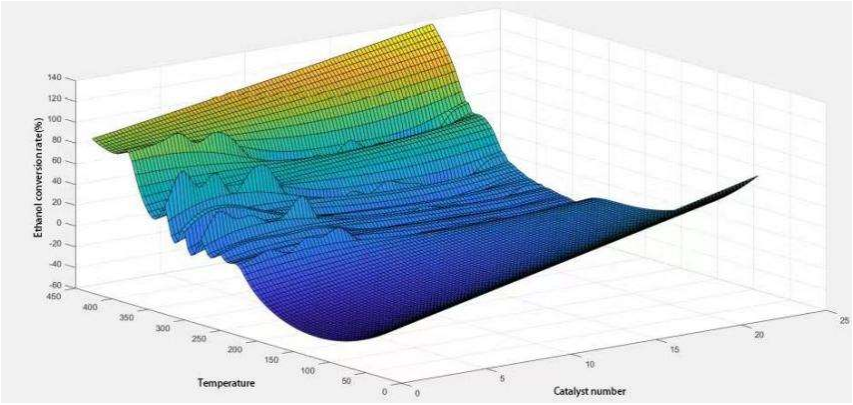

Figure 4. C4 olefin selectivity versus HAP dose and ethanol concentration in three dimensions

The ethanol conversion for each catalyst combination was generally higher than the values at the other reaction temperatures when the temperature was between 350 and 450 °C. These two graphs provide a qualitative analysis of the range of indicators where the maximum values of C4 olefin selectivity and ethanol conversion may be achieved. The range analyzed is less accurate because some of the independent variables do not have as much effect on the dependent variable after superposition as they did before superposition[2]. Therefore, we cannot use the simple control variable method to think about this problem, but need to establish a more complex nonlinear functional relationship to link the five independent variables with the two dependent variables. A neural network model would be good to achieve this goal[3].

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2.3 BP Neural Network Model (BPNN)

The BPNN consists of an input layer, an output layer, and one or more hidden layers. The number of neurons in the input layer is the number of samples, the number of neurons in the hidden layer is usually selected experimentally or based on empirical values, and the number of neurons in the output layer is 1. The learning and training process of the BP algorithm consists of two stages: forward propagation and backward propagation. If the output layer does not get the desired output, it is transferred to the back propagation process, which returns the error signal along the original forward propagation path, and uses the mean square error and gradient descent method to realize the correction of the network connection power to adjust the mean square error value between the actual output of the network and the guidance learning signal[4]. This process is repeated until the specified error requirement is met or the maximum training count is reached and terminated.

2.4 The Basic Process of Neural Network Training

BP neural network through training will make the network has association ability and prediction ability, network training is an important step before model establishment and prediction, its training process of the main steps are shown in Figure 5.

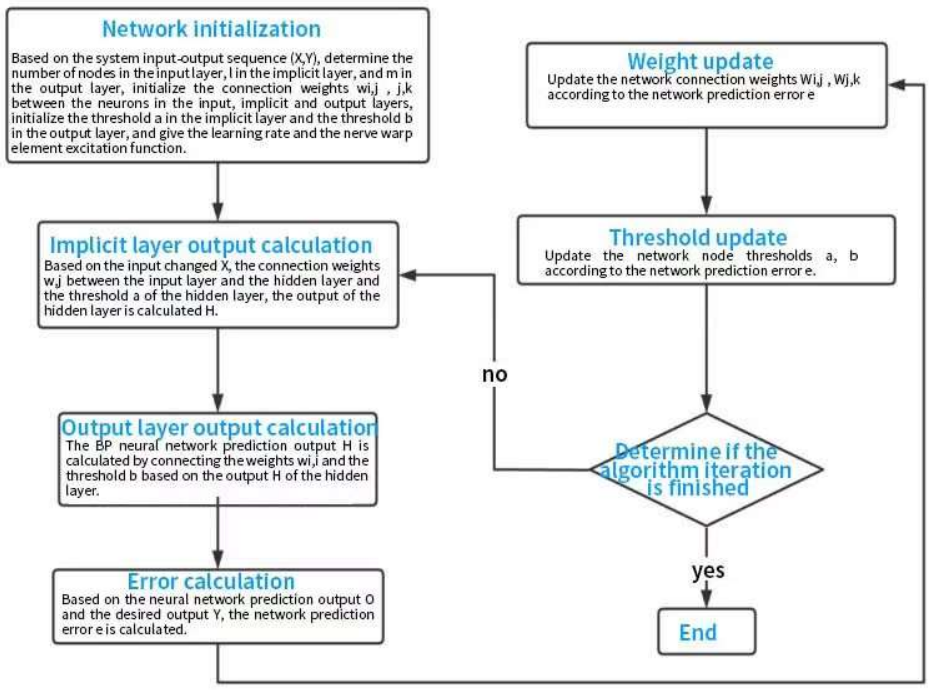

Figure 5. The basic process of neural network training

2.5 A BP Neural Network-based Model for C4 Olefin Selectivity and Ethanol Conversion

The C4 selectivity and ethanol conversion neural network model is used to establish the relationship between Co/SiO2 dose, HAP dose, Co loading, ethanol concentration, and temperature with C4 selectivity and ethanol conversion. Therefore, for this model, the input layer of the neural network has 5 units, which are Co/SiO2 dose, HAP dose, Co loading, ethanol concentration, and temperature; and the output layer has 2 units, which are C4 selectivity and ethanol conversion rate[5]. The reference empirical formula for the number of units in the hidden layer is used to determine the number of hidden layer neurons in the initial network structure, and the optimal number of units in the hidden layer is finally determined after extensive experiments. Where: N1 is the number of input neurons, N2 is the number of output neurons, and N is the number of hidden layer neurons. Therefore, the number of units in the hidden layer is initially set as 2. Based on the above analysis, the C4 selectivity and ethanol conversion rate model of BP neural network is shown in Figure 6.

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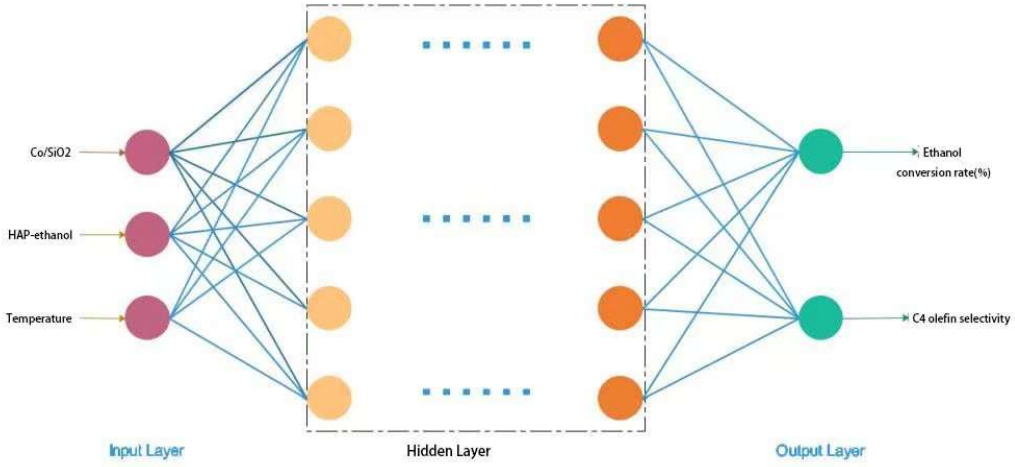

Figure 6. BP neural network model for C4 selectivity and ethanol conversion

2.6 Algorithmic Iterative Solution of Neural Network Models

BP neural network was used to establish a nonlinear function between five indicator factors and C4 selectivity and ethanol conversion. We know that nonlinear mapping capability is an important function of BP neural network, so using this function can achieve some purposes such as function approximation. The number of input vectors and output vectors are determined, and the relationship between them is found by building a BP neural network. the number of neurons in the input layer of the C4 selectivity and ethanol conversion rate model of the BP neural network is 5, and the number of neurons in the output layer is 2. Together with the number of units in the hidden layer determined by the empirical reference formula, the neural network model can be initially established. Based on the previous fitting results, the number of neurons in the hidden layer was continuously adjusted and the error was compared and analyzed to determine the optimal number of neurons in the hidden layer as 10. The final model was set with 75% of the total samples in the training set and 25% of the total samples in the test set, and the conjugate gradient descent training algorithm was used to obtain the model as shown in Figure 7.

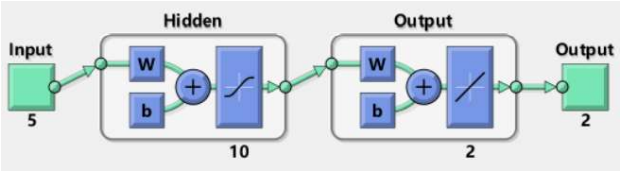

Figure 7. Model Principle

The parameters in the neural network are adjusted with each training session. After more training phases, it was found that the mean square error of the data set was minimized at 58 training cycles, when the model fit was best.

We analyze the results and obtain three conclusions.

The parameters in the neural network are adjusted with each training session. After more training phases, it was found that the mean square error of the data set was the smallest at 58 training cycles, when the model fit was the best.

The goodness-of-fit is all above 0.9, which is close to 1, indicating a better fit.

The orange vertical line in Figure 8 is the zero-error line, and the further away from the line, the larger the error is. It is not difficult to find that the samples in the training, validation and test sets are concentrated in the middle, and the distribution of the two sides is very small, which means that the neural network model is suitable for most of the sample data, and very few of them have large errors.

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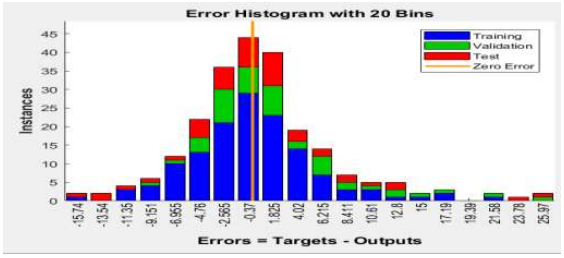

Figure 8. Frequency distribution chart

3. Construction and Solution of 0-1 Planning Model

3.1 Solve for the Optimal Catalyst Combination and Temperature

Since we want to combine all the possibilities in the five indicators of Co/SiO2 dose, HAP dose, Co loading, ethanol concentration, and temperature, a 0-1 planning model can be used for this purpose. The objective function is first established:

$$\max\left(y_1 * y_2\right) \tag{1}$$

(1) in which y1 is the ethanol conversion, y2 is the C4 olefin selectivity, y1*y2 is the C4 olefin yield, and max(y1*y2) is the maximum value of C4 olefin yield.

$$\left[y_1, y_2\right] = f\left(x_1, x_2, x_3, x_4\right) \tag{2}$$

930 where y1 is the ethanol conversion, x1 is the Co/SiO2 dose, x2 is the Co loading, x3 is the HAP dose, x4 is the ethanol concentration, x5 is the reaction temperature, and f(x1,x2,x3,x4,x5) is the neural network model established in Problem 2. This equation will be solved for the combination of the five indicators composition using the neural network model to obtain y1 and y2.

$$p_i = \begin{cases} 1 \\ 0 \end{cases} \tag{3}$$

Pi in (3) is a 0¬1 variable, Pi=1 means that the corresponding indicator data is used as the value of this combination of this indicator, and Pi=0 means that the corresponding indicator data is not used as the value of this combination of this indicator.

$$x_1 = P_1 * 10 + P_2 * 25 + P_3 * 33 + P_4 * 50 + P_5 * 67 + P_6 * 75 + P_7 * 100 + P_8 * 200 \tag{4}$$

(4) The equations P1, P2, P3, P4, P5, P6, P7, P8 indicate whether the Co/SiO2 dose is 10mg,25mg,33mg,50mg,67mg,75mg,100mg,200mg respectively. This equation finally indicates the dose of Co/SiO2 in the combination.

$$x_2 = P_9 * 0.5 + P_{10} * 1 + P_{11} * 2 + P_{12} * 5 \tag{5}$$

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(5) P9, P10, P11, P12 indicate whether the value is taken when the Co loading is 0.5, 1, 2, 5 respectively. This equation finally indicates the value of Co loading in the combination.

$$x_3 = P_{13}*10 + P_{14}*25 + P_{15}*33 + P_{16}*50 + P_{17}*67 + P_{18}*75 + P_{19}*90 + P_{20}*100 + P_{21}*200 \quad (6)$$

(6) P13, P14, P15, P16, P17, P18, P19, P20, P21 indicate whether the value is taken when the HAP dose is 10mg, 25mg, 33mg, 50mg, 67mg, 75mg, 90mg, 100mg, 200mg respectively. This equation finally indicates the dose of HAP in the combination.

$$x_4 = P_{22}*0.3 + P_{23}*0.9 + P_{24}*1.68 + P_{25}*2.1 \quad (7)$$

(7) The equations P21, P22, P23, P24 and P25 indicate whether the value is taken when the ethanol concentration is 0.3ml/min, 0.9ml/min, 1.68ml/min and 2.1ml/min, respectively. This equation finally indicates the value of ethanol concentration in the combination.

$$250 \le x_5 \le 500 \quad (8)$$

Because the catalyst is active in a certain temperature range, this equation indicates the reaction temperature interval of the catalyst combination.

$$P_1 + P_2 + P_3 + P_4 + P_5 + P_6 + P_7 + P_8 = 1 \quad (9)$$

(9) indicates that out of all possible Co/SiO2 doses, one can and can only be chosen.

$$P_9 + P_{10} + P_{11} + P_{12} = 1 \quad (10)$$

(10) indicates that among all possible values of Co loading, one can and can only be chosen.

$$P_{13} + P_{14} + P_{15} + P_{16} + P_{17} + P_{18} + P_{19} + P_{20} + P_{21} = 1 \quad (11)$$

(11) indicates that among all possible HAP doses, only one can be and can be selected.

$$P_{22} + P_{23} + P_{24} + P_{25} = 1 \quad (12)$$

(12) indicates that among all possible values of ethanol concentration, only one can and can be selected.

3.2 Model Solving

Using MATLAB programming, the optimal catalyst combination and temperature were solved to obtain the highest yield of C4 olefins. The results are as follows Table 1.

The highest C4 olefin yield of 63.36% was achieved when the temperature was 500 °C and the catalyst combination was 200 mg5wt% Co/SiO2-100 mgHAP-ethanol concentration 0.30 ml/min and charged in 2-mode.

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Table 1. Optimal catalyst combination and temperature

Co/SiO2 dose	Co load volume	HAP dose	Ethanol concentration	Temperature	C4 olefin absorption rate
200mg	5wt%	100mg	0.30ml/min	500◦C	63.36%

To find the best catalyst combination and temperature that gives the highest yield of C4 olefins when the temperature is below 350 degrees C, we just need to base on the above, with a slight modification in the constraints.

$$250 \leq x_5 \leq 350 \tag{13}$$

Denotes the reaction temperature interval for the required catalyst combination. textbf model was solved for the same using MATLAB programming to obtain the optimal catalyst combination and temperature that resulted in the highest yield of C4 olefins, and the results are shown in Table 2.

Table 2. Optimal catalyst combination and temperature

Co/SiO2 dose	Co load volume	HAP dose	Ethanol concentration	Temperature	C4 olefin absorption rate
200mg	1wt%	10mg	0.30ml/min	350◦C	52.12%

The highest C4 olefin yield of 52.12% was achieved when the temperature was 350 °C and the catalyst combination was 200 mg1wt% Co/SiO2-10 mg HAP-ethanol concentration 0.30 ml/min and charged in 2 mode.

4. Conclusion

In this paper, the interpolation algorithm is used to increase the sample data when the temperature is 325°C before the function fitting, which makes the fitting effect better. And the average of segmented three times Elmit interpolation and three times spline interpolation is used as the interpolation data to ensure the robustness of the data The BP neural network model with strong self-learning and adaptive capability is used to avoid the inaccurate analysis results caused by the simple control variable method. 0-1 planning model is compatible with the actual catalyst inputs, and is more general and generalizable for such combinatorial class problems. However, since the sample data are too small, and the more data the BP neural network model has, the better the fitting effect is, so the established model may still have room for optimization.

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