Process optimization of C4 olefins by ethanol coupling based on BP neural network and genetic algorithm

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Abstract. C4 olefins are widely used in chemical production, and the preparation of C4 olefins by ethanol coupling is one of the important methods to obtain this raw material, so it is important to study the process conditions for the preparation of C4 olefins. In this paper, we analyze and discuss the correlation between catalyst combination and temperature on ethanol conversion and C4 olefin selectivity based on the experimental data collected from laboratory preparation, and explore the reasonable catalyst combination scheme and temperature selection in order to achieve the optimization of preparation efficiency. Further investigation of the preparation process to obtain the optimum yield is also carried out based on the error of the validation results.

Keywords: Optimal catalyst combination; BP neural network; Average impact value; Genetic algorithm.

1. Introduction

C4 olefins are common raw materials in chemical production, and ethanol is an easily accessible clean energy source and a major raw material for the preparation of C4 olefins. Among the preparation processes, temperature control and catalyst selection are important factors affecting the selectivity of C4 olefins and their yields. To ensure the efficiency of C4 olefin preparation, the selection of reasonable temperature and catalyst combination is of great research significance. Therefore, the degree of influence of catalyst combination and temperature on the conversion of ethanol, and the selectivity of C4 olefins was studied to explore the multi-factor relationship. On this basis, the catalyst combination and temperature were optimized to maximize the experimental C4 olefin yield, and the catalyst combination and temperature were further optimized according to the temperature limitation conditions.

2. Model Assumptions and Notation

2.1. Assumptions

1. When investors consider each investment choice, it is base 1. All experimental data are valid experimental data and there are no experimental anomalies.
2. It is assumed that all experimental results conform to some probability distribution.
3. It is assumed that there are no other factors influencing the experimental results.

2.1.1 Notations

Important notations used in this paper are listed in TABLE 1.

Table 1. Notations

Symbols	Description
τ	Kendall correlation coefficient
P	Corresponding matrix
Z	Transition Matrix
R	Line profile distribution function
C	Column profile distribution function

3. Model construction and solving

3.1. The degree of influence of multiple factors on the selectivity of C4 olefins

3.1.1 Introduction to BP Neural Networks

BP (backpropagation) neural network is a concept proposed by scientists led by Rumelhart and McClelland in 1986, is a multi-layer feedforward neural network trained according to the error backpropagation algorithm, so it is also known as backpropagation neural network, through the training of sample data, constantly correct the network weights and thresholds so that the error function along the negative gradient direction down, approximating the desired output, BP neural network is one of the most widely used neural networks[1].

3.1.2 BP neural network construction and structure

In this paper, seven indicators in the input layer were selected to represent A/B loading method, Co/SiO2 weight, Co loading, Co/SiO2 and HAP loading ratio, catalyst carrier category, ethanol concentration and temperature, and the output layer was ethanol conversion and C4 olefin selectivity results, and the experimental data were used to construct a BP neural network in order to complete the analysis of correlation later.

The feedforward neural network was constructed in MATLAB, and the appropriate training algorithm and activation function were selected [2]. The activation function is an important tool to complete the flow process of data from one form to another, from one dimension to another, and realize the flow process of data from data layer to final output layer. The activation function here is selected as a linear function and a hyperbolic 10 tangent S-shaped function. The expression of the activation function is.

$$f(x) = x \tag{1}$$

$$\tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}} \tag{2}$$

As shown in Fig. 1, the training was stopped after 1000 iterations using MATLAB language, and a single hidden layer with 13 activation elements in the hidden layer was trained as a BP neural network with MSE of order of 10-6, which meets the error requirement.

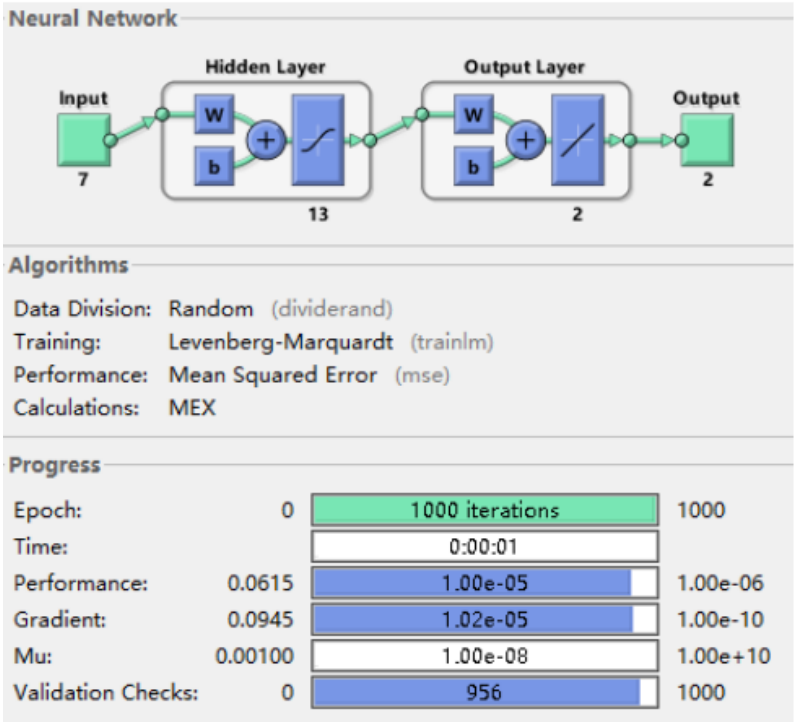


Fig 1. Neural network structure diagram and result performance

3.1.3 Average impact value and calculation

MeanImpactValue (MIV) is considered one of the best indicators for evaluating the correlation of variables in neural networks, and the main operation is to input the independent variables into the neural network, and by the resulting output layer data, the corresponding calculation is performed to derive the MIV value, and the magnitude of the impact is compared by the absolute value of the MIV value [3,4].

The catalyst data were first processed and the catalyst combinations were finely split into five categories. They were divided into A/B loading method, Co/SiO2 weight, Co loading, Co/SiO2 and HAP loading ratio, and catalyst carrier category (quartz sand/HAP).

The independent and dependent variables were selected to construct a suitable BP neural network. Temperature and ethanol concentration plus the six catalysts after splitting constituted the seven independent variables, and ethanol conversion and C4 olefin selectivity constituted the two dependent variables.

Each set of independent variables was increased by 10% to form vector A and decreased by 10% to form vector B, and then brought into the generated BP neural network.

The result IV (impactvalue) of A-B is obtained, which indicates the impact value of the change of the independent variable on the output. Finally, the IV is averaged by the number of observed cases to obtain the corresponding variable MIV of the independent variable, and then the absolute value of MIV is taken and compared for the same result to obtain the ranking of the impact of each variable on the result. MIV values for each indicator is shown in Table 2. Analysis of the weight contribution of MIV is shown in Fig. 2.

Table 2. MIV values for each indicator

	Effect on ethanol conversion rate	Effect on the selectivity of C4 olefins
A/B loading method	0.0030	0.1269
Co/SiO2 Weight	0.1361	0.0787
Co load capacity	0.0633	0.0247
Co/SiO2 and carrier charge ratio	0.1223	0.0824
Catalyst carrier category	0.0921	0.2503
Ethanol concentration	0.0438	0.0206
Temperature	0.5395	0.4164

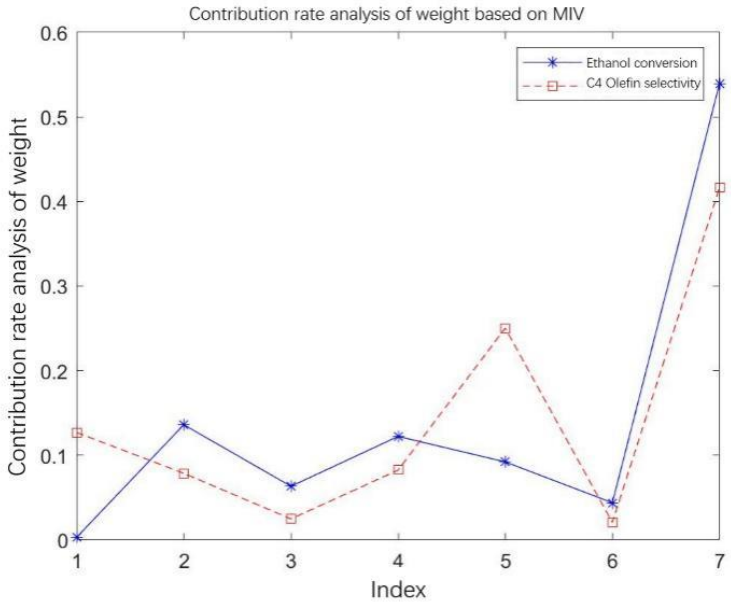


Fig 2. Analysis of the weight contribution of MIV

3.1.4 Analysis of results

From the above figure and the above table, it can be concluded that the most influential factor on ethanol conversion and C4 olefin selectivity is temperature. Among the influencing factors of ethanol conversion, except for the temperature factor, the more important index is Co/SiO2 weight, and the loading method almost has no effect on ethanol conversion. Among the factors affecting C4 olefins, except for temperature, the catalyst carrier type had a greater influence, while ethanol concentration and Co loading had a smaller influence.

3.2. Optimization of catalyst combination and temperature

3.2.1 Introduction to Genetic Algorithms

Genetic algorithm, is an algorithmic model that simulates the iterative evolution of organisms in nature. The algorithm directly calculates the fitting results without considering the properties of the fitted curve such as derivability, concavity, and continuity, while the high independence makes it easy to combine with some curve fitting algorithms and stochastic evolution to avoid falling into local optimum, so it is suitable for the extreme value solving problem of numerical fitting of artificial neural networks [5].

3.2.2 Genetic algorithm optimization: no temperature constraints

Firstly, the catalyst combination was deconstructed and the process conditions such as catalyst combination and temperature were split into a total of seven indicators, and each sample was input to the neural network as a seven-dimensional vector, and the final output of C4 olefin yield was obtained [6-8].

As shown in Fig. 3, a single hidden layer with 13 activation elements in the hidden layer was trained as a BP neural network using MATLAB language after 139 iterations, and the MSE was in the order of 10-9, which meets the error requirement. The fitting effect is shown in Fig. 4, and the trained neural network performs well on the overall sample.

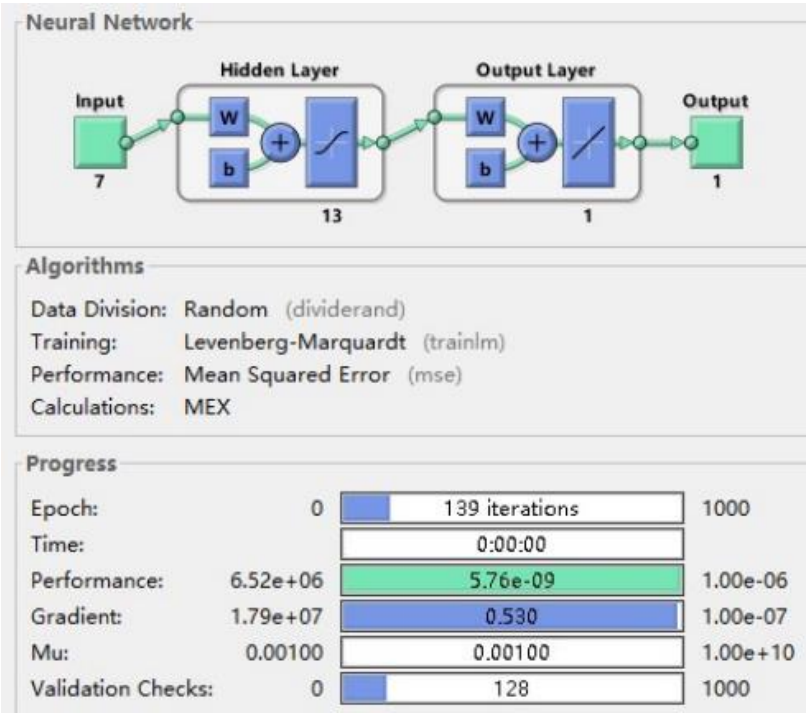


Fig 3. New BP neural network structure and training results

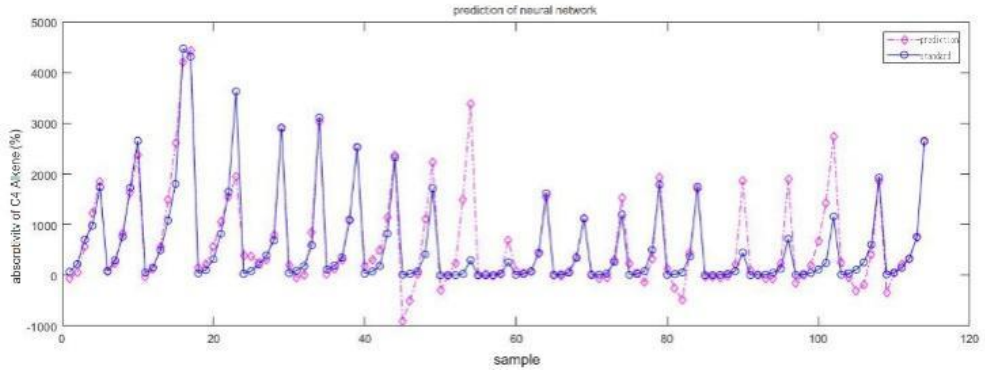


Fig 4. Fitting of the new BP neural network on the overall sample

After the neural network training is completed, the genetic algorithm is used to find the optimal solution that makes the objective function take the maximum value. Setting the number of evolutionary generations as 300, the initial population size as 50, the crossover probability as 0.5, and the variation probability as 0.02, the maximum value of the function is obtained as 0.8621, and the process condition of the corresponding optimal solution is shown in Fig. 5. A/B loading method is A; Co/SiO2 weight is 67mg; Co loading is 6.55Wt%; Co/SiO2 and carrier loading ratio is 0.78; catalyst carrier type is HAP; ethanol concentration is 4.07ml/min; temperature is 499.

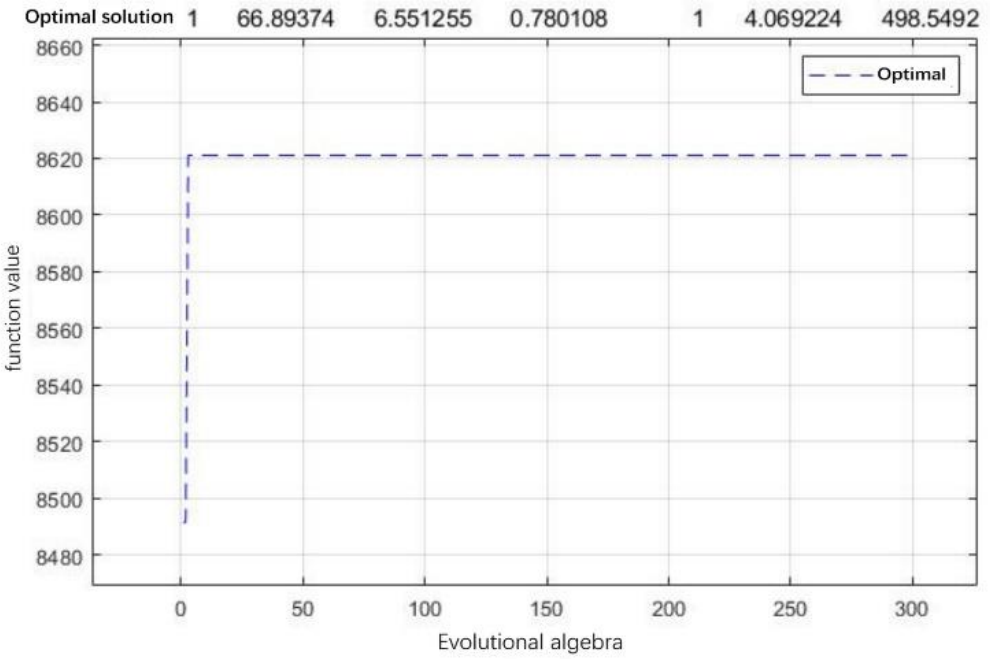


Fig 5. Diagram of the iterative process of the optimal solution

3.2.3 Genetic Algorithm Solution: Temperature Constraints

Following the same steps [9], we continued to investigate the optimal process conditions for the preparation of C4 olefins by ethanol coupling at temperatures below 350 degrees. Using the above neural network model and genetic algorithm model, setting the temperature definition domain not higher than 350[10], the evolutionary results were obtained as shown in Fig. 6, and the maximum value under the solution restriction was 0.7515. A/B loading method is B; Co/SiO2 weight is 82mg; Co loading is 6Wt%; Co/SiO2 and carrier loading ratio is 0.837; catalyst carrier category is 1; ethanol concentration is 9.57ml/min; temperature is 345.

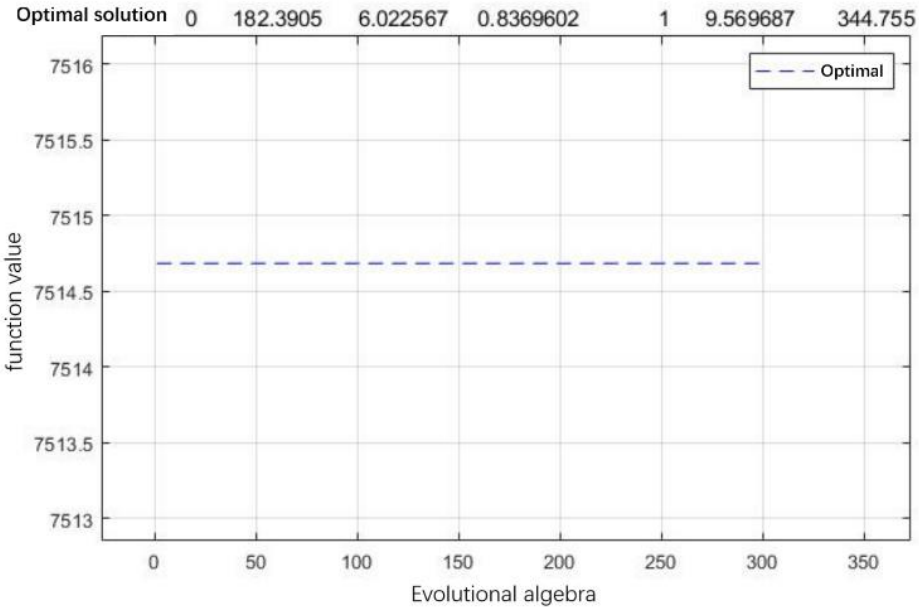


Fig 6. Optimal solution iteration process Figure 2

4. Conclusion

In this paper, we first used a BP neural network prediction model to obtain the predicted values of ethanol conversion and C4 olefin selectivity after inputting catalyst combination and temperature, where catalyst combination was subdivided into several indicators such as loading method, Co loading, Co/SiO2 weight, Co/SiO2 and HAP loading ratio, catalyst carrier type, and ethanol concentration. Since we mainly focused on the degree of influence of the catalyst combination and temperature indicators in the prediction process, we used the mean impact value (MIV) method to calculate the weight magnitude of each indicator, which is considered as one of the best methods to evaluate the correlation of variables in neural networks. We calculated and compared the absolute magnitude of the MIV values using the predicted values of ethanol conversion and C4 olefin selectivity. The analysis of the results shows that the most influential factor on both ethanol conversion and C4 olefin selectivity is temperature. In addition to the temperature factor, the more important index for ethanol conversion was Co/SiO2 weight, and the more important factor for C4 olefins was the catalyst carrier type.

After obtaining the weights of each influencing factor, we continued to explore the optimal conditions for C4 olefin preparation. In this experiment, we chose to use genetic algorithms to find the maximum C4 olefin yield under two conditions, without and with temperature range limitation, so as to obtain the corresponding process conditions. The corresponding bp neural network was trained based on the two conditions to obtain the corresponding C4 olefin yield. After several iterations of genetic inheritance, the optimal yield was found to be 0.8621 under the condition of no temperature range limitation, which corresponds to the process conditions in Table 6, and the optimal yield was found to be 0.7515 under the condition of temperature range limitation below 350, which corresponds to the process conditions in Table 7.

References

[1] Yang, Liu. Research on wind-electricity-thermal correlation analysis method based on Copula function [D]. Northeastern Electric Power University, 2020.

[2] Zhu Xinling. Correlation coefficient and Copula function correlation [J]. Journal of Wuhan University of Science and Technology, 2009, 32(06): 664-668.

[3] LIN Wei, ZHAO He, HAO Yiwen, ZHU Zongping, RAO Ya-shu, ZHAO Hai-liang, KOKO Xin, ZHAO Xuan, LIAO Wan. Dose correlation of Chai Hu-Bai Shao pair in the treatment of "liver depression and blood deficiency" based on Copula function[J]. Chinese herbal medicine, 2021, 52(13): 4007-4013.

[4] Zhou Ying. Research on rolling bearing fault diagnosis technology based on MIV feature screening and BP neural network [D]. Beijing Jiaotong University, 2011..

[5] Jiang, Q., Huang, R., Huang, Y., Chen, S., He, Y., Lan, L., & Liu, C. (2019). Application of BP neural network based on genetic algorithm optimization in evaluation of power grid investment risk. IEEE Access, 7, 154827-154835.

[6] Katoch, S., Chauhan, S. S., & Kumar, V. A review on genetic algorithm: past, present, and future [J]. Multimedia Tools and Applications, 2021, 80(5): 8091-8126.

[7] Mo-Meng, Zhao-Long-Zhang, Gong-oi-Wen, Wu-Yang. Research application of BP neural network based on genetic algorithm optimization [J]. Modern Electronics Technology, 2018, 41(9): 41-4.

[8] Hu K, Luo WP, Jia Shulin. Octane prediction model based on BP neural network [J]. Journal of Wuhan Textile University, 2021, 34(04): 27-32.

[9] Lv Shaopei. Preparation of butanol and C4 olefins by ethanol coupling. [D]. Dalian: Dalian University of Technology, 2018.

[10] Karimi, Asadollah, Hadi Soltani, and Aydin Hasanzadeh. An analysis of increasing the purity of ethylene production in the ethylene fractionation column by the genetic algorithm [J]. Chemical Product and Process Modeling, 2020; 15(3): 20190088.