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Research on C4 Olefin Yield Optimization Based on BP Neural Network and Single Objective Optimization

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Abstract: *In this paper, the effects of different catalyst combinations and temperatures on ethanol conversion rate and C4 olefin selectivity in the reaction of preparing C4 olefins by ethanol coupling are mainly studied, and the optimal reaction conditions for maximizing C4 olefin yield are found according to the established model. A single-objective optimization model was established with the total weight of catalyst, Co loading, Co/SiO2 and HAP loading ratio, ethanol concentration and temperature as independent variables and C4 olefin yield as dependent variables. Then, neural network model is used to predict C4 olefin yield data under different influencing factors, and genetic algorithm is used to find the optimal solution.*

Keywords: *Single Objective Optimization; BP Neural Network; Genetic Algorithm*

1. Introduction

C4 olefin is an important raw material of chemical products and medicines, and its traditional production methods all depend on fossil energy. However, with the continuous development of society, the shortage of fossil energy and the environmental problems brought by its transformation and application become more and more obvious, so it has become urgent to find a green, sustainable and alternative new energy source to prepare C4 olefin. Among the many alternative energy sources, ethanol has been widely concerned by researchers because of its advantages of wide sources, easy conversion and little pollution. [1]

Although remarkable achievements have been made in the research of coupling conversion of ethanol to C4 olefins, the combination of catalysts (Co loading, Co/SiO2 and HAP loading ratio, ethanol concentration) and temperature will affect the selectivity and yield of C4 olefins, and other products such as ethylene and acetaldehyde will inevitably be produced. [2]

2. Prediction Model of C4 Olefin Yield Based on BP Neural Network

In order to quantitatively study the relationship between the reaction conditions and the catalytic results, the reaction conditions are mainly described by five index variables: total catalyst mass, Co loading, mass ratio of Co/SiO2 and HAP, ethanol concentration, and temperature. Catalytic results are described by ethanol conversion multiplied by C4 olefin selectivity.

According to the analysis, except for the temperature variable, other indicators have strong discreteness. The establishment of multiple regression model will have the disadvantages of over-fitting and large deviation, so here we choose BP neural network model to predict C4 olefin yield corresponding to any set of indicators, [3] The specific process is as follows:

The five index variables of total catalyst, Co loading, mass ratio of Co/SiO2 and HAP, ethanol concentration and temperature are named x1-x5 respectively, and the ethanol conversion rate and C4 olefin selectivity are named y1 and y2, then the C4 olefin yield is equal to y1 * y2.

Establish the model of BP neural network, as shown in Figure 1, the input layer is x1-x5, and the output layer is y1 and y2;

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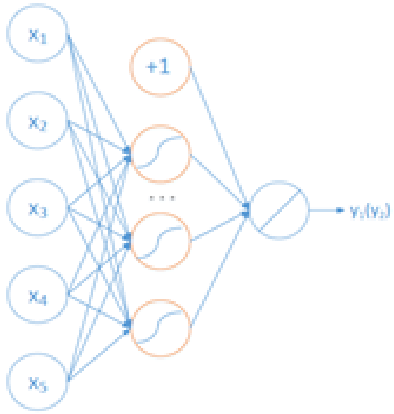

Figure 1: BP neural network model

We set the number of nodes in the hidden layer to 10, and the function of the hidden layer is tansig type. Its expression and image are shown in the figure below. The nonlinear activation function can keep the original proportional relationship of the input layer data after multiple Sigmoid transformations.

$$y = tan\,sig\,(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \tag{1}$$

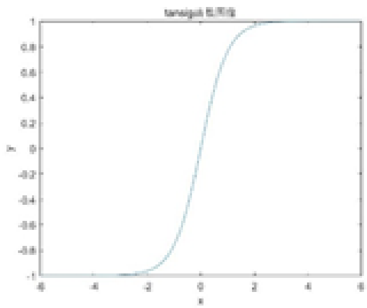

Figure 2: Tansig function image

After the model is established, 109 combinations of index variables x1~x5 in Annex I and y1 and y2 corresponding to each combination are taken as learning samples, which are input into the neural network out of order for training. Its learning rule is to use the steepest descent method to continuously adjust the weights and thresholds of the network through back propagation, so as to minimize the sum of square errors of the network and obtain the best results. The schematic diagram of the learning process is shown in Figure 3.

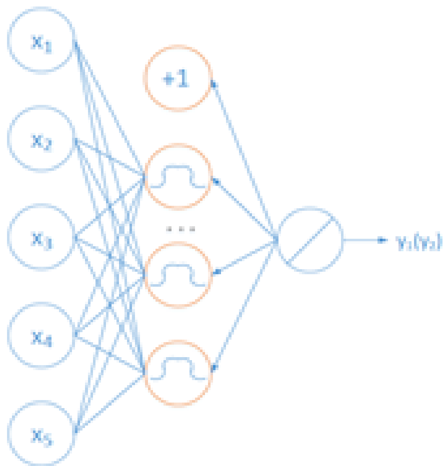

Figure 3: Neural Network Back Propagation Update Weight

The learning results are shown in Figure 4.

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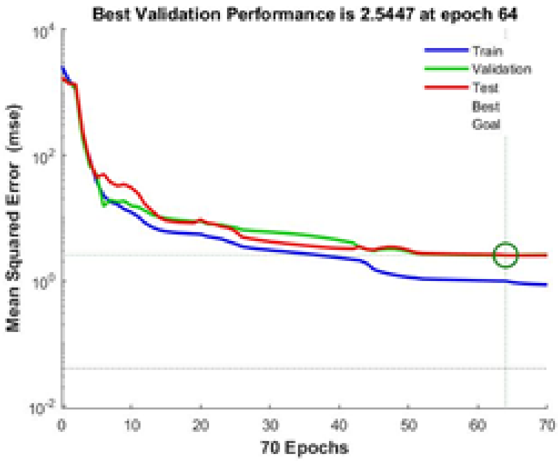

Figure 4: Neural network learning results

It can be seen that after 64 steps of learning, the final convergence error of the neural network model is 100, which is 2.5447.

After learning, for the combination of catalyst and temperature index that is not in the data, after inputting it into neural network, the ethanol conversion rate and C4 olefin selectivity can be predicted, and the predicted C4 olefin yield corresponding to this combination can be obtained by multiplying them.

3. The C4 olefin yield maximization Model Based on Single Objective Optimization

In order to search for the index combination that can maximize the yield of C4 olefins, a single objective optimization model is established. [4] The objective function is min=y1*y2, and the independent variables are x1, x2, x3, x4, X5; Because these five index variables can't be infinitely increased or decreased in the reaction, it is necessary to define their ranges. Their range of change is defined in the range from the minimum value to the maximum value of each index in the data, and the final model is as follows:

$$max\, y\,1 \cdot y2 \tag{2}$$

$$s.t.\begin{cases} 20 \le x1 \le 400 \\ 0.5 \le x2 \le 5 \\ 0.5 \le x3 \le 2 \\ 0.3 \le x4 \le 2.1 \\ 250 \le x5 \le 450 \end{cases} \tag{3}$$

Theoretically, it is only necessary to exhaust all possible combinations within the range of change and predict the corresponding C4 olefin yield according to neural network, and screen out the maximum yield and the corresponding combination. However, even under the condition of limited scope, it is still time-consuming and laborious to exhaustively calculate the five-dimensional array corresponding to five index variables, so consider using genetic algorithm, one of the intelligent swarm algorithms, to discuss this problem. [5]

(1) coding: the mapping from phenotype to genotype is called coding, and here we use decimal coding. The five index variables are regarded as genes, and their gene codes are decimal values of variables, which are still within the previously specified range.

(2) Generation of initial population: through formula

$$rand * (Gmax - Gmin) + Gmin \tag{4}$$

$Gmax$ is the maximum of gene range, $Gmin$ is the minimum of gene range, corresponding genes are randomly generated, and by this method, N individuals are randomly generated, with N=100, forming an initial population, referred to as population for short, and evolving from generation to generation until the optimal solution of the problem is generated.

(3) Evaluation of fitness value: the fitness function is mainly used to judge whether each individual or solution is good or bad, that is, the greater the fitness value, the greater the probability of inheritance to the next generation, and vice versa. The fitness function is: according to individual genes, the trained

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neural network is predicted to get y1 and y2 respectively, and y1*y2 is regarded as the fitness function, that is, the objective function is

$$max\, y\,1 \cdot y2 \tag{5}$$

(4) Selection: select some excellent individuals from the T-generation population and pass them on to the next generation population.

(5) crossover: each individual in the group is valued in (0,1) by using the rand function, and when the probability is less than 0.2, crossover operation is performed on the individual, and then the values are again valued in (0,1) by using the rand function, and the values are passed through the matlab code Flov (RAND * (n-1)). Map the random number to each individual in the population, take the value in (0,1) by using the rand function again, and map the random number to the number of nodes in the gene by using the matlab code floov(rand*(5-1)), and cross the two ends of this node.

(6) Mutation: For each gene of each individual in the population, use the rand function to take a value in (0,1). When the random number is less than 0.2, it is considered to be a mutation operation, and then use the rand function to take a value in (0,1) again. If the random number is less than 0.5, it is considered to reduce the gene, otherwise, it is considered to increase the gene. The formula gi * (1-rand * (1-t/100)) is used for mapping, where t is the iteration number, and we set the iteration number t to 100 times in order to save time, so as to obtain a better solution.

Through the above steps, the yield of C4 olefins is as high as possible when the total amount of catalyst, the loading of Co, the mass ratio of Co/SiO2 and HAP, and the concentration of ethanol are 400mg, 1.83wt%, 1.9, 0.9ml/min and 400℃.

When the temperature is lower than 350℃, change the constraint condition to:

$$max\, y\,1 \cdot y2 \tag{6}$$

$$s.t.\begin{cases} 20 \le x1 \le 400 \\ 0.5 \le x2 \le 5 \\ 0.5 \le x3 \le 2 \\ 0.3 \le x4 \le 2.1 \\ 250 \le x5 \le 450 \\ T \le 350℃ \end{cases} \tag{7}$$

The genetic algorithm is also used to optimize, and it is found that when the total amount of catalyst, Co loading, mass ratio of Co/SiO2 and HAP, ethanol concentration and temperature are 400mg, 0.5wt%, 0.6, 0.9ml/min and 350℃, the yield of C4 olefins is as high as possible.

The known data of ethanol conversion rate and C4 olefin selectivity to be predicted, and the corresponding total amount of catalyst, Co load, ethanol concentration and temperature are taken as training samples to predict the charging ratio of Co/Sio2 and HAP, and to explore whether the known charging ratio of Co/Sio2 and HAP is consistent with the predicted charging ratio of Co/Sio2 and HAP. Because the essence of neural network prediction is a kind of regression, the predicted values of Co/Sio2 and HAP charge ratios are not discrete values, but continuous values. We classify them by neural network. When the predicted values of Co/Sio2 and HAP charge ratios are less than 0.9, it is considered that the Co/Sio2 and HAP charge ratios are 0.5, and when the Co/Sio2 and HAP charge ratios are greater than 0.9, and the Co/Sio2 and HAP charge ratios are 0.5. In other cases, the charge ratio of Co/Sio2 and HAP is 2. Randomly select ten data to judge whether the classification result predicted by neural network is the same as the original data, and the correct rate is 90%.

4. Conclusion

In this paper, it is an optimization problem to study the catalyst combination and temperature setting mode that can make C4 olefin yield as high as possible. Firstly, considering the performance index data in the data, the multivariate nonlinear fitting analysis was carried out, and it was determined that the total weight of catalyst, Co loading, Co/SiO2 and HAP loading ratio, ethanol concentration and temperature were independent variables, and ethanol conversion rate and C4 olefin selectivity were multivariate functions of dependent variables. However, in the known data, only the temperature changes continuously from 250 degrees to 400 degrees, while the data of other indexes are all discretely changed, so the function fitted by these data will have the disadvantages of over-fitting and large deviation. Therefore, the neural network prediction model is established. By training the existing data repeatedly,

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the network can predict the corresponding values of ethanol conversion rate and C4 olefin selectivity according to the index variable data that are not provided in the input data, and the C4 olefin yield corresponding to the input data can be obtained by multiplying them.

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