ISSN 2616-5767 Vol.5, Issue 6: 55-57, DOI: 10.25236/AJETS.2022.050610

Exploration of process conditions for coupling C4 olefins based on neural network prediction model

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Abstract: *In today's rapidly developing economy, industrial development is increasingly being updated. C4 olefins are widely used as important chemical raw materials in the production of chemicals and pharmaceuticals, and ethanol is the main raw material for the production of C4 olefins. Investigating the process conditions for the catalytic coupling of ethanol to C4 olefins has great environmental and economic value. Therefore, in this paper, a BP neural network prediction model is used to fit and predict the experimental data based on existing chemical experiments to obtain the optimal process conditions for the highest possible yield of C4 olefins.*

Keywords: *Neural network prediction, C4 olefin, Process conditions*

1. Introduction

In today's context, human civilisation has entered the fourth industrial revolution. As an important organic chemical raw material, C4 olefins are now widely used in chemical and pharmaceutical production, and ethanol is one of the raw materials for the production of C4 olefins. The wide range of products involved in the conversion of ethanol results in low selectivity and poor economics of the target product. At the same time, catalyst combinations (Co loading, Co/SiO2 and HAP charge ratios, ethanol concentration combinations) and temperature have an impact on the selectivity and C4 olefin harvesting rate, so the design of catalyst combinations with different ratios is of great environmental and economic value to explore the optimal process conditions for the catalytic coupling of ethanol to C4 olefins.

2. Model Establishment and Solution

2.1. BP Neural Network Prediction Model

The BP neural network model is a model that approximates the desired output by training on sample data and continuously modifying the network weights and thresholds so that the error function decreases in the negative step direction. the topology of the BP neural network model consists of an input layer, an implicit layer and an output layer.

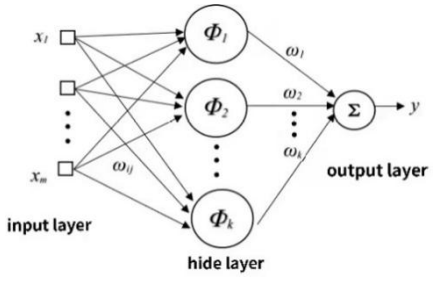

Figure 1: Topology of BP Neural Network Model

A neural network can be seen as a function mapping for problems where there is a clear correspondence between input and output, but where the function is not easily determined. The prediction of C4 olefin yield can be seen as a complex function mapping problem with Co/SiO2, HAP, ethanol concentration and temperature as inputs and C4 olefin yield as outputs. Therefore, BP neural network can be used as the prediction of C4 olefin yield.

Step 1: Calculate the C4 olefin yield from the previous experimental data using an excel spreadsheet

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and ascend the order to obtain the catalyst combinations and temperatures from low to high yield.

Step 2: Referring to the catalyst combinations and temperatures with higher yields in the excel data, the catalyst and temperature parameters were adjusted to set up another four sets of process conditions that were experimentally proposed to give higher C4 olefin yields, and the C4 olefin yields were predicted by a BP neural network model.

Step 3: The 114 different process condition combinations and the calculated C4 olefin yields were imported into MATLAB as learning training samples for machine learning.

Step 4: The trained neural network model is used to predict the four sets of simulations set up to obtain the yield of C4 olefins under the corresponding process conditions.

2.2. Data Fitting and Training

The four catalyst combinations with the highest C4 olefin yields, all in the range of 3000-4000, were obtained by calculating and adjusting the excel spreadsheet experimental data in ascending order, weighing the results and setting up four additional experiments with different process conditions that could result in higher yields and making neural network predictions.

Co/SiO2	HAP(mg)	Ethanol concentration (ml/min)	Temperature(℃)	C4 olefin yield
10	200	1.68	400	3111.366512
1	200	1.68	400	3627.781909
2	200	0.9	450	4311.844167
2	200	0.9	400	4472.805978
simulation experiment				
2	200	0.9	400	
1	200	0.9	450	
2	200	1.68	400	
2	200	0.9	450	

Figure 2: Simulation Experiment

The data from 114 samples were imported into MATLAB and the levenberg marquardt algorithm for neural networks was used to train the experimental combinations. four samples of Co/SiO2, HAP, ethanol concentration and temperature were used as input variables and the C4 olefin yield samples were used as output variables.

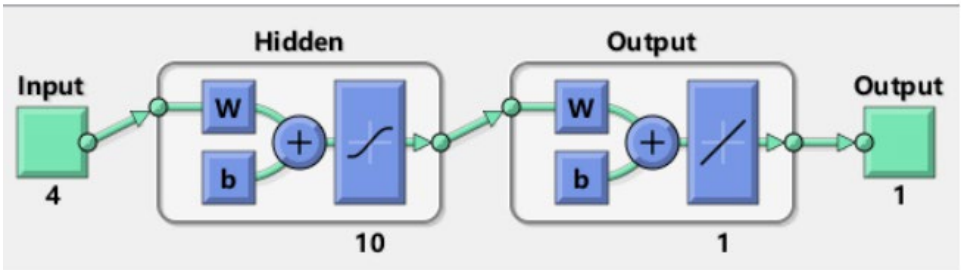

Figure 3: BP Neural Network Structure

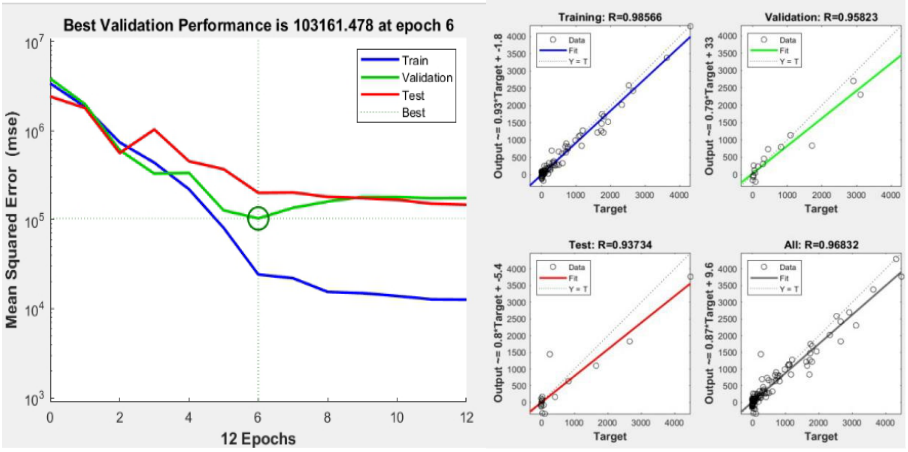

Figure 4: BP Neural Network Fitting Effect

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After 12 iterations of the neural network the optimal fit was plotted. The mean squared error of the best validation group was minimized at the sixth fit, and MATLAB regressed the true and fitted values to obtain a goodness of fit R greater than 0.9, indicating that the BP neural network was a good predictor of the yield of ethanol coupled with C4 olefins.

2.3. Neural network prediction results

The trained neural network model was used to predict the yield of C4 olefins under the corresponding process conditions from four sets of simulated experiments. The highest yield of C4 olefin was found to be 4294 for the 200 mg 1 wt% Co/SiO2- 200 mg HAP- 0.9 ml/min ethanol concentration and 450 °C. The other three combinations also gave yields in the range of 3000-4000. This is consistent with previous chemical experiments which concluded that the optimum conditions for the reaction of ethanol coupling to prepare C4 olefins should be that the best C4 olefin yield is achieved when 1Co/SiO2-HAP is mixed 1:1 with HAP and the optimum reaction temperature for C4 olefins over the catalyst is 400°C. This leads to the conclusion that exploring the optimal process conditions for the catalytic coupling of ethanol for the preparation of C4 olefins can be predicted by simulation using a machine learning BP neural network model.

simulation experiment			Neural network prediction results	
Co/SiO2	HAP(mg)	Ethanol concentration (ml/min)	Temperature(℃)	C4 olefin yield
2	200	0.9	400	3766.2
1	200	0.9	450	4255.1
2	200	1.68	400	3689.4
2	200	0.9	450	4294

Figure 5: Prediction Effect of Catalyst Combination

3. Model Evaluation

This paper uses the neural network prediction of machine learning. After measuring the gray correlation model and the neural network, utilizing select machine learning is the best way because it is simple to operate, and the prediction result can form a large number of samples which can be obtained in a short time. During future chemical experiments, utilizing machine learning can reduce the number of experiments, reduce the use of raw materials and get optimal programming.

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